

PMID- 26967682

OWN - NLM

STAT- In-Data-Review

DA - 20160419

IS - 1520-4898 (Electronic)

IS - 0001-4842 (Linking)

VI - 49

IP - 4

DP - 2016 Apr 19

TI - μ -Nitrido Diiron Macrocyclic Platform: Particular Structure for Particular Catalysis.

PG - 583-93

LID - 10.1021/acs.accounts.5b00458 [doi]

AB - The ultimate objective of bioinspired catalysis is the development of efficient and clean chemical processes. Cytochrome P450 and soluble methane monooxygenase enzymes efficiently catalyze many challenging reactions. Extensive research has been performed to mimic their exciting chemistry, aiming to create efficient chemical catalysts for functionalization of strong C-H bonds. Two current biomimetic approaches are based on (i) mononuclear metal porphyrin-like complexes and (ii) iron and diiron non-heme complexes. However, biomimetic catalysts capable of oxidizing CH₄ are still to be created. In the search for powerful oxidizing catalysts, we have recently proposed a new bioinspired strategy using N-bridged diiron phthalocyanine and porphyrin complexes. This platform is particularly suitable for stabilization of Fe(IV)Fe(IV) complexes and can be useful to generate high-valent oxidizing active species. Indeed, the possibility of charge delocalization on two iron centers, two macrocyclic ligands, and the nitrogen bridge makes possible the activation of H₂O₂ and peracids. The ultrahigh-valent diiron-oxo species (L)Fe(IV)-N-Fe(IV)(L(+*)) horizontal lineO (L = porphyrin or phthalocyanine) have been prepared at low temperatures and characterized by cryospray MS, UV-vis, EPR, and Mossbauer techniques. The highly electrophilic (L)Fe(IV)-N-Fe(IV)(L(+*)) horizontal lineO species exhibit remarkable reactivity. In this Account, we describe the catalytic applications of μ -nitrido diiron complexes in the oxidation of methane and benzene, in the transformation of aromatic C-F bonds under oxidative conditions, in oxidative dechlorination, and in the formation of C-C bonds. Importantly, all of these reactions can be performed under mild and clean conditions with high conversions and turnover numbers. μ -Nitrido diiron species retain their binuclear structure during catalysis and show the same mechanistic features (e.g., (18)O labeling, formation of benzene epoxide, and NIH shift in aromatic oxidation) as the enzymes operating via high-valent iron-oxo species. μ -Nitrido diiron complexes can react with perfluorinated aromatics under oxidative conditions, while the strongest oxidizing enzymes cannot. Advanced spectroscopic, labeling, and reactivity studies have confirmed the involvement of high-valent diiron-oxo species in these catalytic reactions. Computational studies have shed light on the origin of the remarkable catalytic properties, distinguishing the Fe-N-Fe scaffold from Fe-C-Fe and Fe-O-Fe analogues. X-ray absorption and emission spectroscopies assisted with DFT calculations allow deeper insight into the electronic structure of these

particular complexes. Besides the novel chemistry involved, iron phthalocyanines are cheap and readily available in bulk quantities, suggesting high application potential. A variety of macrocyclic ligands can be used in combination with different transition metals to accommodate M-N-M platform and to tune their electronic and catalytic properties. The structural simplicity and flexibility of mu-nitrido dimers make them promising catalysts for many challenging reactions.

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LA - eng

PT - Journal Article

DEP - 20160311

PL - United States

TA - Acc Chem Res

JT - Accounts of chemical research

JID - 0157313

SB - IM

EDAT- 2016/03/12 06:00

MHDA- 2016/03/12 06:00

CRDT- 2016/03/12 06:00

PHST- 2016/03/11 [aheadofprint]

AID - 10.1021/acs.accounts.5b00458 [doi]

PST - ppublish

SO - Acc Chem Res. 2016 Apr 19;49(4):583-93. doi: 10.1021/acs.accounts.5b00458. Epub 2016 Mar 11.

PMID- 26926185

OWN - NLM

STAT- In-Data-Review

DA - 20160323

IS - 1944-8252 (Electronic)

IS - 1944-8244 (Linking)

VI - 8

IP - 11

DP - 2016 Mar 23

TI - Self-Assembled Monolayers of Perfluoroanthracenylaminoalkane Thiolates on Gold as Potential Electron Injection Layers.

PG - 7308-19

LID - 10.1021/acsami.6b00532 [doi]

AB - As a material with relatively small band gap and low lying valence orbitals, perfluoroanthracene (PFA) is of interest for the modification of electrode

surfaces, for example, as charge injection layers for n-type organic semiconductors. To covalently attach PFA in the form of self-assembled monolayers (SAMs), we developed a synthesis of derivatives with a sulfur termination, linked to the 2-position of the PFA moieties by an -NH- group and a short alkane chain with two and three methylene groups, respectively. Spectroscopic characterization of the SAMs reveals that the molecules adopt an almost upright orientation on the gold surface, with the packing density mostly determined by the steric demands of the PFA units. The number of the methylene groups in the -NH-alkyl linker has only a minor impact on the SAM structure because of the nonsymmetric attachment of the PFA units, which permits the compensation of the orientational constraints imposed by the bending potential. The investigated SAMs alter the work function of gold by $+(0.59-0.64)$ eV, suggesting comparably strong depolarization effects, affecting the extent of the work function modification.

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LA - eng

PT - Journal Article

DEP - 20160309

PL - United States

TA - ACS Appl Mater Interfaces

JT - ACS applied materials & interfaces

JID - 101504991

SB - IM

OTO - NOTNLM

OT - band gap

OT - organic electronics

OT - perfluorinated arenes
 OT - self-assembled monolayers
 OT - work function
 EDAT- 2016/03/02 06:00
 MHDA- 2016/03/02 06:00
 CRDT- 2016/03/02 06:00
 PHST- 2016/03/09 [aheadofprint]
 AID - 10.1021/acsami.6b00532 [doi]
 PST - ppublish
 SO - ACS Appl Mater Interfaces. 2016 Mar 23;8(11):7308-19. doi:
 10.1021/acsami.6b00532. Epub 2016 Mar 9.

 PMID- 26790871
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160303
 IS - 1618-2650 (Electronic)
 VI - 408
 IP - 8
 DP - 2016 Mar
 TI - A fast method for analysing six perfluoroalkyl substances in human serum by
 solid-phase extraction on-line coupled to liquid chromatography tandem mass
 spectrometry.
 PG - 2159-70
 LID - 10.1007/s00216-016-9319-0 [doi]
 AB - We have developed and validated an on-line TurboFlow solid-phase extraction
 procedure coupled to high-performance liquid chromatography with tandem mass
 spectrometry for the analysis of six perfluoroalkyl substances (PFAS), two
 sulfonates (perfluorooctane sulfonate and perfluorohexane sulfonate), three
 carboxylates (perfluorooctanoic acid, perfluorononanoic acid and
 perfluorodecanoic acid), and one sulfonamide (N-methylperfluorooctane
 sulfonamide), in human serum samples. This method requires only 100 µL of sample
 and involves a short pre-treatment with acetonitrile followed by addition of a
 labelled internal standard for quantification and ultracentrifugation. All PFAS
 were detected with a run time of 8.5 min. Linearity ranges stay between 0.1 and
 20 µg L⁻¹ (R² > 0.9960). Recoveries were determined by spiking blank serum
 samples with a mixture of six PFAS and found to be in the range 96-110 % for all
 compounds. Isotopic dilution was used to quantify the selected analytes. The low
 limits of quantification obtained, between 0.16 and 0.34 µg L⁻¹, small volume
 of sample required and short run time used (from two to three times shorter than
 any other described method), make this validated method highly recommended for
 human biomonitoring studies. Graphical Abstract System solid phase extraction on
 line coupled LC-MS/MS to analyse six perfluoroalkyl substances in human serum.
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LA - eng

PT - Journal Article

DEP - 20160120

PL - Germany

TA - Anal Bioanal Chem

JT - Analytical and bioanalytical chemistry

JID - 101134327

SB - IM

OTO - NOTNLM

OT - Human biomonitoring

OT - Human serum

OT - Liquid chromatography with tandem spectrometry

OT - On-line solid-phase extraction

OT - Perfluoroalkyl substances

OT - Turbo flow extraction

EDAT- 2016/01/23 06:00

MHDA- 2016/01/23 06:00

CRDT- 2016/01/22 06:00

PHST- 2015/10/15 [received]

PHST- 2016/01/07 [accepted]

PHST- 2015/12/19 [revised]

PHST- 2016/01/20 [aheadofprint]

AID - 10.1007/s00216-016-9319-0 [doi]

AID - 10.1007/s00216-016-9319-0 [pii]

PST - ppublish

SO - Anal Bioanal Chem. 2016 Mar;408(8):2159-70. doi: 10.1007/s00216-016-9319-0. Epub 2016 Jan 20.

PMID- 26985970

OWN - NLM

STAT- In-Data-Review

DA - 20160406

IS - 1520-6882 (Electronic)
IS - 0003-2700 (Linking)
VI - 88
IP - 7
DP - 2016 Apr 5
TI - Screening of Toxic Chemicals in a Single Drop of Human Whole Blood Using Ordered Mesoporous Carbon as a Mass Spectrometry Probe.
PG - 4107-13
LID - 10.1021/acs.analchem.6b00444 [doi]
AB - Surface-enhanced laser desorption/ionization (SELDI) is a versatile and high-throughput mass spectrometry (MS) technique that uses a probe for extraction, enrichment, desorption, and ionization of target analytes. Here we report ordered mesoporous carbon as a new SELDI probe for rapid screening and identification of trace amount of toxic chemicals in a single drop of human whole blood without complicated sample preparation procedures. We demonstrate that ordered mesoporous carbon not only can selectively enrich a wide variety of low-mass toxic compounds from whole blood samples but also can be used as an excellent matrix to assist the laser desorption/ionization process of small molecules with low background noise, high repeatability, and good salt tolerance. High sensitivity (detection limits at ppt levels) and good reproducibility for typical toxic compounds were obtained. With CMK-8 as a SELDI probe, we successfully identified and screened six perfluorinated compounds in a single drop of whole blood collected from workers in a perfluorochemical plant. The method was also validated with complex samples such as human urine and environmental water samples. With distinct advantages such as simplicity, rapidness, minimal sample requirement, and high reliability, this method keeps great promise for various aspects of application.
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 LA - eng
 PT - Journal Article
 DEP - 20160324
 PL - United States
 TA - Anal Chem
 JT - Analytical chemistry
 JID - 0370536
 SB - IM
 EDAT- 2016/03/18 06:00
 MHDA- 2016/03/18 06:00
 CRDT- 2016/03/18 06:00
 PHST- 2016/03/24 [aheadofprint]
 AID - 10.1021/acs.analchem.6b00444 [doi]
 PST - ppublish
 SO - Anal Chem. 2016 Apr 5;88(7):4107-13. doi: 10.1021/acs.analchem.6b00444. Epub 2016 Mar 24.

 PMID- 27058923
 OWN - NLM
 STAT- Publisher
 DA - 20160408
 LR - 20160409
 IS - 1879-1514 (Electronic)
 IS - 0166-445X (Linking)
 VI - 175
 DP - 2016 Mar 31
 TI - PFOS, PFNA, and PFOA sub-lethal exposure to embryonic zebrafish have different toxicity profiles in terms of morphometrics, behavior and gene expression.
 PG - 160-170
 LID - S0166-445X(16)30090-X [pii]
 LID - 10.1016/j.aquatox.2016.03.026 [doi]
 AB - Polyfluorinated compounds (PFC) are a class of anthropogenic, persistent and toxic chemicals. PFCs are detected worldwide and consist of fluorinated carbon

chains of varying length, terminal groups, and industrial uses. Previous zebrafish studies in the literature as well as our own studies have shown that exposure to these chemicals at a low range of concentrations (0.02-2.0µM; 20-2000ppb) resulted in chemical specific developmental defects and reduced post hatch survival. It was hypothesized that sub-lethal embryonic exposure to perfluorooctanesulfonic acid (PFOS), perfluorononanoic acid (PFNA), or perfluorooctanoic acid (PFOA) would result in different responses with regard to morphometric, behavior, and gene expression in both yolk sac fry and larval zebrafish. Zebrafish were exposed to PFOS, PFOA, and PFNA (0.02, 0.2, 2.0µM) for the first five days post fertilization (dpf) and analyzed for morphometrics (5 dpf, 14 dpf), targeted gene expression (5 dpf, 14 dpf), and locomotive behavior (14 dpf). All three PFCs commonly resulted in a decrease in total body length, increased *tfc3a* (muscle development) expression and decreased *apls* (protein transport) expression at 5dpf, and hyperactive locomotor activity 14 dpf. All other endpoints measured at both life-stage time points varied between each of the PFCs. PFOS, PFNA, and PFOA exposure resulted in significantly altered responses in terms of morphometric, locomotion, and gene expression endpoints, which could be manifested in field exposed teleosts.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20160331

TA - Aquat Toxicol

JT - Aquatic toxicology (Amsterdam, Netherlands)

JID - 8500246

OTO - NOTNLM

OT - Danio rerio

OT - Morphometrics

OT - PFNA

OT - PFOA

OT - PFOS
 OT - Zebrafish locomotion
 EDAT- 2016/04/09 06:00
 MHDA- 2016/04/09 06:00
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 PHST- 2016/02/26 [received]
 PHST- 2016/03/29 [revised]
 PHST- 2016/03/30 [accepted]
 AID - S0166-445X(16)30090-X [pii]
 AID - 10.1016/j.aquatox.2016.03.026 [doi]
 PST - aheadofprint
 SO - Aquat Toxicol. 2016 Mar 31;175:160-170. doi: 10.1016/j.aquatox.2016.03.026.

 PMID- 27015565
 OWN - NLM
 STAT- Publisher
 DA - 20160325
 LR - 20160326
 IS - 1879-1514 (Electronic)
 IS - 0166-445X (Linking)
 VI - 175
 DP - 2016 Mar 10
 TI - Response of Lemna minor L. to short-term cobalt exposure: The effect on
 photosynthetic electron transport chain and induction of oxidative damage.
 PG - 117-126
 LID - S0166-445X(16)30062-5 [pii]
 LID - 10.1016/j.aquatox.2016.03.009 [doi]
 AB - The effect of two concentrations of cobalt (Co²⁺) on photosynthetic activity and
 antioxidative response in Lemna minor L. were assessed 24, 48 and 72h after the
 start of the exposure. Higher concentration of cobalt (1mM) induced growth
 inhibition while lower concentration (0.01mM) increased photosynthetic pigments
 content. Analysis of chlorophyll a fluorescence transients revealed high
 sensitivity of photosystem II primary photochemistry to excess of Co²⁺ especially
 at the higher concentration where decreased electron transport beyond primary
 quinone acceptor QA- and impaired function of oxygen evolving complex (OEC) was
 observed. Due to impairment of OEC, oxygen production was decreased at higher
 Co²⁺ concentration. Activity of superoxide dismutase was mainly inhibited while
 lipid peroxidation increased, at both concentrations, indicating that
 cobalt-induced oxidative damage after short exposure and moreover, susceptibility
 of the membranes in the cell to cobalt toxicity. Results obtained in this study
 suggest possible application of used parameters as tools in assessment of early
 damage caused by metals.
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LA - ENG
PT - JOURNAL ARTICLE
DEP - 20160310
TA - Aquat Toxicol
JT - Aquatic toxicology (Amsterdam, Netherlands)
JID - 8500246
OTO - NOTNLM
OT - Cobalt
OT - Lemna minor
OT - Lipid peroxidation
OT - Oxygen evolving complex
OT - Photosystem II
EDAT- 2016/03/26 06:00
MHDA- 2016/03/26 06:00
CRDT- 2016/03/26 06:00
PHST- 2015/04/09 [received]
PHST- 2016/03/03 [revised]
PHST- 2016/03/08 [accepted]
AID - S0166-445X(16)30062-5 [pii]

AID - 10.1016/j.aquatox.2016.03.009 [doi]

PST - aheadofprint

SO - Aquat Toxicol. 2016 Mar 10;175:117-126. doi: 10.1016/j.aquatox.2016.03.009.

PMID- 26749332

OWN - NLM

STAT- In-Data-Review

DA - 20160225

IS - 1434-3916 (Electronic)

IS - 0936-8051 (Linking)

VI - 136

IP - 3

DP - 2016 Mar

TI - Prophylactic augmentation of the proximal femur: an investigation of two techniques.

PG - 345-51

LID - 10.1007/s00402-015-2400-x [doi]

AB - INTRODUCTION: Osteoporotic hip fractures are an increasing problem in an ageing population. They result in high morbidity, mortality and high socioeconomic costs. For patients with poor bone quality, prophylactic augmentation of the proximal femur might be an option for fracture prevention. METHODS: In two groups of paired human femora the potential of limited polymethyl-methacrylate (PMMA) augmentation (11-15 ml) in a V-shape pattern and the insertion of a proximal femur nail antirotation (PFNA) blade were investigated. The testing was carried out pair wise simulating the single leg stand. The untreated femur in each pair served as control. An axial load was applied until failure. Load displacement parameters and temperature increase during the augmentation process were recorded. RESULTS: In the PMMA group no significant difference was found between the augmented and non-augmented specimen concerning load to failure ($p = 0.35$) and energy to failure ($p = 0.9$). A median temperature increase of 9.5 degrees C was observed in the augmented specimen. A significant correlation was found between the amount of applied PMMA and the temperature increase (Cor. Coef. = 0.82, $p = 0.042$). In the PFNA group, a significant decrease of load to failure and a non-significant decrease of energy to failure were observed ($p = 0.037$ and $p = 0.075$). CONCLUSION: Limited V-shaped PMMA augmentation and PFNA blade insertion did not show any improvement in failure load or energy to failure. Volumes of up to 15 ml PMMA did not cause a critical surface temperature increase.

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LA - eng

PT - Journal Article

DEP - 20160109

PL - Germany

TA - Arch Orthop Trauma Surg

JT - Archives of orthopaedic and trauma surgery

JID - 9011043

SB - IM

OTO - NOTNLM

OT - Cement augmentation

OT - Hip Fracture

OT - Osteoporosis

OT - Single leg stand

EDAT- 2016/01/11 06:00

MHDA- 2016/01/11 06:00

CRDT- 2016/01/11 06:00

PHST- 2015/02/09 [received]

PHST- 2016/01/09 [aheadofprint]

AID - 10.1007/s00402-015-2400-x [doi]

AID - 10.1007/s00402-015-2400-x [pii]

PST - ppublish

SO - Arch Orthop Trauma Surg. 2016 Mar;136(3):345-51. doi: 10.1007/s00402-015-2400-x. Epub 2016 Jan 9.

PMID- 25827101

OWN - NLM

STAT- In-Data-Review

DA - 20160216

LR - 20160226

IS - 1432-0738 (Electronic)

IS - 0340-5761 (Linking)

VI - 90

IP - 3

DP - 2016 Mar

TI - Programming of metabolic effects in C57BL/6JxFVB mice by in utero and lactational exposure to perfluorooctanoic acid.

PG - 701-15

LID - 10.1007/s00204-015-1488-7 [doi]

AB - Perfluorooctanoic acid (PFOA) is known to cause developmental toxicity and is a suggested endocrine disrupting compound (EDC). Early life exposure to EDCs has been implicated in programming of the developing organism for chronic diseases

later in life. Here we study perinatal metabolic programming by PFOA using an experimental design relevant for human exposure. C57BL/6JxFVB hybrid mice were exposed during gestation and lactation via maternal feed to seven low doses of PFOA at and below the NOAEL used for current risk assessment (3-3000 microg/kg body weight/day). After weaning, offspring were followed for 23-25 weeks without further exposure. Offspring showed a dose-dependent decrease in body weight from postnatal day 4 to adulthood. Growth under high fat diet in the last 4-6 weeks of follow-up was increased in male and decreased in female offspring. Both sexes showed increased liver weights, hepatic foci of cellular alterations and nuclear dysmorphology. In females, reductions in perigonadal and perirenal fat pad weights, serum triglycerides and cholesterol were also observed. Endocrine parameters, such as glucose tolerance, serum insulin and leptin, were not affected. In conclusion, our study with perinatal exposure to PFOA in mice produced metabolic effects in adult offspring. This is most likely due to disrupted programming of metabolic homeostasis, but the assayed endpoints did not provide a mechanistic explanation. The BMDL of the programming effects in our study is below the current point of departure used for calculation of the tolerable daily intake.

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LA - eng
PT - Journal Article
DEP - 20150401
PL - Germany
TA - Arch Toxicol
JT - Archives of toxicology
JID - 0417615
SB - IM
PMC - PMC4754331
OID - NLM: PMC4754331
OTO - NOTNLM
OT - Developmental exposure
OT - Endocrine disrupting compounds
OT - Metabolic effects
OT - Perfluorooctanoic acid
OT - Programming
EDAT- 2015/04/02 06:00
MHDA- 2015/04/02 06:00
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PHST- 2014/09/18 [received]
PHST- 2015/02/23 [accepted]
PHST- 2015/04/01 [aheadofprint]
AID - 10.1007/s00204-015-1488-7 [doi]
AID - 10.1007/s00204-015-1488-7 [pii]
PST - ppublish
SO - Arch Toxicol. 2016 Mar;90(3):701-15. doi: 10.1007/s00204-015-1488-7. Epub 2015 Apr 1.

PMID- 25588985
OWN - NLM
STAT- In-Data-Review
DA - 20160216
IS - 1432-0738 (Electronic)
IS - 0340-5761 (Linking)
VI - 90
IP - 3
DP - 2016 Mar
TI - Perfluorononanoic acid in combination with 14 chemicals exerts low-dose mixture effects in rats.
PG - 661-75
LID - 10.1007/s00204-015-1452-6 [doi]
AB - Humans are simultaneously exposed to several chemicals that act jointly to induce mixture effects. At doses close to or higher than no-observed adverse effect levels, chemicals usually act additively in experimental studies. However, we are lacking knowledge on the importance of exposure to complex real-world mixtures at more relevant human exposure levels. We hypothesised that adverse mixture effects occur at doses approaching high-end human exposure levels. A mixture (Mix) of 14

chemicals at a combined dose of 2.5 mg/kg bw/day was tested in combination with perfluorononanoic acid (PFNA) at doses of 0.0125 (Low PFNA), 0.25 (Mid PFNA) and 5 (High PFNA) mg/kg bw/day by oral administration for 14 days in juvenile male rats. Indication of a toxicokinetic interaction was found, as simultaneous exposure to PFNA and the Mix caused a 2.8-fold increase in plasma PFNA concentrations at Low PFNA. An increase in testosterone and dihydrotestosterone plasma concentrations was observed for Low PFNA + Mix. This effect was considered non-monotonic, as higher doses did not cause this effect. Reduced LH plasma concentrations together with increased androgen concentrations indicate a disturbed pituitary-testis axis caused by the 15-chemical mixture. Low PFNA by itself increased the corticosterone plasma concentration, an effect which was normalised after simultaneous exposure to Mix. This combined with affected ACTH plasma concentrations and down-regulation of 11beta HSD mRNA in livers indicates a disturbed pituitary-adrenal axis. In conclusion, our data suggest that mixtures of environmental chemicals at doses approaching high-end human exposure levels can cause a hormonal imbalance and disturb steroid hormones and their regulation. These effects may be non-monotonic and were observed at low doses. Whether this reflects a more general phenomenon that should be taken into consideration when predicting human mixture effects or represents a rarer phenomenon remains to be shown.

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LA - eng
PT - Journal Article
DEP - 20150115
PL - Germany
TA - Arch Toxicol
JT - Archives of toxicology
JID - 0417615
SB - IM
OTO - NOTNLM
OT - Corticosterone
OT - Mixture toxicology
OT - Perfluorononanoic acid (PFNA)
OT - Pituitary hormones
OT - Steroidogenesis
OT - Testosterone
EDAT- 2015/01/16 06:00
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PHST- 2015/01/15 [aheadofprint]
AID - 10.1007/s00204-015-1452-6 [doi]
AID - 10.1007/s00204-015-1452-6 [pii]
PST - ppublish
SO - Arch Toxicol. 2016 Mar;90(3):661-75. doi: 10.1007/s00204-015-1452-6. Epub 2015 Jan 15.

PMID- 26978125
OWN - NLM
STAT- In-Data-Review
DA - 20160324

IS - 1757-6199 (Electronic)
IS - 1757-6180 (Linking)
VI - 8
IP - 7
DP - 2016 Apr
TI - Polar stir bars for isolation and preconcentration of perfluoroalkyl substances from human milk samples prior to UHPLC-MS/MS analysis.
PG - 633-47
LID - 10.4155/bio-2015-0009 [doi]
AB - BACKGROUND: A new method for the determination of four perfluoroalkyl carboxylic acids (from C5 to C8) and perfluorooctane sulfonate in human milk samples using stir-bar sorptive extraction-ultra-HPLC-MS/MS has been accurately optimized and validated. METHODOLOGY: Polydimethylsiloxane and polyethyleneglycol modified silicone materials were evaluated. DISCUSSION: Overall, polyethyleneglycol led to a better sensitivity. After optimizing experimental variables, the method was validated reaching detection limits in the range of 0.05-0.20 ng ml⁻¹; recovery rates from 81 to 105% and relative standard deviations fewer than 13% in all cases. The method was applied to milk samples from five randomly selected women. All samples were positive for at least one of the target compounds with concentrations ranging between 0.8 and 6.6 ng ml⁻¹, being the most abundant perfluorooctane sulfonate.
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LA - eng
PT - Journal Article
DEP - 20160315

PL - England
TA - Bioanalysis
JT - Bioanalysis
JID - 101512484
SB - IM
OTO - NOTNLM
OT - UHPLC-MS/MS
OT - endocrine disrupting chemicals
OT - human milk
OT - perfluoroalkyl substances
OT - sample preparation
OT - stir-bar sorptive extraction
EDAT- 2016/03/16 06:00
MHDA- 2016/03/16 06:00
CRDT- 2016/03/16 06:00
PHST- 2016/03/15 [aheadofprint]
AID - 10.4155/bio-2015-0009 [doi]
PST - ppublish
SO - Bioanalysis. 2016 Apr;8(7):633-47. doi: 10.4155/bio-2015-0009. Epub 2016 Mar 15.

PMID- 26850367

OWN - NLM

STAT- In-Data-Review

DA - 20160316

IS - 1520-4812 (Electronic)

IS - 1043-1802 (Linking)

VI - 27

IP - 3

DP - 2016 Mar 16

TI - Divalent Amino-Acid-Based Amphiphilic Antioxidants: Synthesis, Self-Assembling Properties, and Biological Evaluation.

PG - 772-81

LID - 10.1021/acs.bioconjchem.6b00002 [doi]

AB - We report herein the synthesis of a divalent amphiphilic carrier onto which alpha-phenyl-N-tert-butyl nitron (PBN) and 6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid (Trolox) antioxidants were grafted to give the divalent derivative called FATxPBN. The divalent carrier consists of two lysine amino acids as a scaffold upon which the antioxidant moieties are grafted, a perfluorinated chain that supplies hydrophobicity, and a sugar-based polar headgroup that ensures water solubility. For the sake of comparison, a divalent PBN derivative called FADiPBN was also synthesized. The self-aggregation properties of FATxPBN and FADiPBN were studied by means of surface tension, dynamic light scattering, and transmission electron microscopy methods, and showed they form small micelles (i.e., 12 and 6 nm diameter, respectively) at submillimolar concentrations (i.e., 0.01 and 0.05 mM, respectively), in agreement with partition coefficient values. The superior antioxidant properties of FATxPBN over FADiPBN and the parent compounds PBN and Trolox were demonstrated using in vitro ABTS(*+) reduction (98%) and soybean

lipoxygenase inhibition (94%) assays. Finally, FATxPBN was found to significantly inhibit hyperglycemia-induced toxicity on an ex-vivo rat model, demonstrating its potency as a bioactive antioxidant against oxidative stress-induced damage.

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LA - eng

PT - Journal Article

DEP - 20160222

PL - United States

TA - Bioconjug Chem

JT - Bioconjugate chemistry

JID - 9010319

SB - IM

EDAT- 2016/02/07 06:00
 MHDA- 2016/02/07 06:00
 CRDT- 2016/02/07 06:00
 PHST- 2016/02/22 [aheadofprint]
 AID - 10.1021/acs.bioconjchem.6b00002 [doi]
 PST - ppublish
 SO - Bioconj Chem. 2016 Mar 16;27(3):772-81. doi: 10.1021/acs.bioconjchem.6b00002.
 Epub 2016 Feb 22.

PMID- 26893124
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160303
 IS - 1364-548X (Electronic)
 IS - 1359-7345 (Linking)
 VI - 52
 IP - 21
 DP - 2016 Mar 3
 TI - Synthesis of quaternary alpha-perfluoroalkyl lactams via electrophilic perfluoroalkylation.
 PG - 4049-52
 LID - 10.1039/c6cc00700g [doi]
 AB - Efficient protocols enabling the rapid installation of trifluoromethyl, as well as further functionalized fluoroalkyl groups by an electrophilic perfluoroalkylation of lactam-derived ketene silyl amides (KSAs) using hypervalent iodine reagents 1 and 2 have been developed.
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 LA - eng
 PT - Journal Article
 PL - England
 TA - Chem Commun (Camb)
 JT - Chemical communications (Cambridge, England)
 JID - 9610838
 SB - IM
 EDAT- 2016/02/20 06:00
 MHDA- 2016/02/20 06:00
 CRDT- 2016/02/20 06:00
 AID - 10.1039/c6cc00700g [doi]
 PST - ppublish
 SO - Chem Commun (Camb). 2016 Mar 3;52(21):4049-52. doi: 10.1039/c6cc00700g.

PMID- 26969042
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160422
 IS - 1528-0691 (Electronic)
 IS - 1528-0691 (Linking)
 VI - 16
 IP - 2
 DP - 2016 Apr
 TI - Synthesis of Organofluoro Compounds Using Methyl Perfluoroalk-2-ynoates as Building Blocks.
 PG - 907-23
 LID - 10.1002/tcr.201500258 [doi]
 AB - This review provides an overview of several synthetic applications of methyl perfluoroalk-2-ynoates, leading to convenient preparation of many perfluoroalkylated compounds. The use of these important substrates in the synthesis of various five-, six-, and seven-membered heterocycles, cyclopentadienes, and biphenyls is described, alongside a discussion of the mechanistic aspects of these reactions.
 CI - (c) 2016 The Chemical Society of Japan & Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim.
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LA - eng
PT - Journal Article
DEP - 20160310
PL - United States
TA - Chem Rec
JT - Chemical record (New York, N.Y.)
JID - 101085550
SB - IM
OTO - NOTNLM
OT - Michael addition
OT - drug design
OT - fluorine
OT - perfluoroalkyl groups
OT - synthetic methods
EDAT- 2016/03/13 06:00
MHDA- 2016/03/13 06:00
CRDT- 2016/03/13 06:00
PHST- 2015/10/20 [received]
PHST- 2016/03/10 [aheadofprint]
AID - 10.1002/tcr.201500258 [doi]
PST - ppublish
SO - Chem Rec. 2016 Apr;16(2):907-23. doi: 10.1002/tcr.201500258. Epub 2016 Mar 10.

PMID- 26617289
OWN - NLM
STAT- In-Data-Review
DA - 20160310

IS - 1521-3765 (Electronic)

IS - 0947-6539 (Linking)

VI - 22

IP - 12

DP - 2016 Mar 14

TI - Incremental Tuning Up of Fluorous Phenazine Acceptors.

PG - 3930-6

LID - 10.1002/chem.201504122 [doi]

AB - In a simple, one-step direct trifluoromethylation of phenazine with CF₃ I we prepared and characterized nine (poly)trifluoromethyl derivatives with up to six CF₃ groups. The electrochemical reduction potentials and gas-phase electron affinities show a direct, strict linear relation to the number of CF₃ groups, with phenazine(CF₃)₆ reaching a record-high electron affinity of 3.24 eV among perfluoroalkylated polyaromatics.

CI - (c) 2016 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.

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 PT - Journal Article
 DEP - 20160112
 PL - Germany
 TA - Chemistry
 JT - Chemistry (Weinheim an der Bergstrasse, Germany)
 JID - 9513783
 SB - IM
 OTO - NOTNLM
 OT - azaacenes
 OT - electrochemistry
 OT - electron affinity
 OT - semiconductors
 OT - trifluoromethyl groups
 EDAT- 2015/12/01 06:00
 MHDA- 2015/12/01 06:00
 CRDT- 2015/12/01 06:00
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 PHST- 2016/01/12 [aheadofprint]
 AID - 10.1002/chem.201504122 [doi]
 PST - ppublish
 SO - Chemistry. 2016 Mar 14;22(12):3930-6. doi: 10.1002/chem.201504122. Epub 2016 Jan 12.

 PMID- 26933840
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160420
 IS - 1521-3765 (Electronic)
 IS - 0947-6539 (Linking)
 VI - 22
 IP - 18
 DP - 2016 Apr 25
 TI - Photocatalytic/Cu-Promoted C-H Activations: Visible-light-Induced ortho-Selective Perfluoroalkylation of Benzamides.
 PG - 6218-22
 LID - 10.1002/chem.201600229 [doi]
 AB - A visible-light-induced and copper-promoted perfluoroalkylation of benzamides was successfully developed under the assistance of an 8-aminoquinoline directing group. It provides a straightforward method for the synthesis of ortho-perfluoroalkyl-substituted benzoic acid derivatives. The reaction employs a cheap organic dye eosin Y as the photoredox catalyst and is run under the irradiation of a 26 W fluorescent LED light bulb.

CI - (c) 2016 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.
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 LA - eng
 PT - Journal Article
 DEP - 20160316
 PL - Germany
 TA - Chemistry
 JT - Chemistry (Weinheim an der Bergstrasse, Germany)
 JID - 9513783
 SB - IM
 OTO - NOTNLM
 OT - Cu-promoted
 OT - C-H activation
 OT - chelation-assisted
 OT - perfluoroalkylation
 OT - photocatalysis
 EDAT- 2016/03/05 06:00

MHDA- 2016/03/05 06:00
 CRDT- 2016/03/03 06:00
 PHST- 2016/01/18 [received]
 PHST- 2016/03/16 [aheadofprint]
 AID - 10.1002/chem.201600229 [doi]
 PST - ppublish
 SO - Chemistry. 2016 Apr 25;22(18):6218-22. doi: 10.1002/chem.201600229. Epub 2016 Mar 16.

 PMID- 26945239
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160323
 IS - 1879-1298 (Electronic)
 IS - 0045-6535 (Linking)
 VI - 151
 DP - 2016 May
 TI - Annual dynamics of perfluorinated compounds in sediment: A case study in the Morava River in Zlin district, Czech Republic.
 PG - 225-33
 LID - 10.1016/j.chemosphere.2016.02.081 [doi]
 LID - S0045-6535(16)30241-7 [pii]
 AB - Two groups of perfluorinated compounds (PFCs), i.e. perfluoroalkyl sulfonates (PFASs) and perfluoroalkyl carboxylates (PFCAs) were analysed during a period of 1 year in monthly collected riverbed sediment samples from five sampling sites in an industrial region in Morava River catchment in Czech Republic. Levels of PFCs determined in sediment samples were up to 6.8 µg kg⁻¹ of dry weight. Among PFCs analysed, mainly short-chain PFASs (C6 to C8) including PFOS were found in sediment samples and their levels were similar to those found in comparable river basins in other parts of Europe. Concentrations of PFCs were correlated with organic carbon content and their variations were mainly correlated by high flow events on Morava River and its tributaries. The changes in PFC concentrations were induced by displacing of PFCs containing particles to the river sediment during these elevated flow events.
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 LA - eng
 PT - Journal Article
 DEP - 20160315
 PL - England
 TA - Chemosphere
 JT - Chemosphere
 JID - 0320657
 SB - IM
 OTO - NOTNLM
 OT - Monitoring
 OT - PFOS
 OT - Perfluorinated compounds
 OT - Sediment
 OT - Water
 OT - Water framework directive
 EDAT- 2016/03/06 06:00
 MHDA- 2016/03/06 06:00
 CRDT- 2016/03/06 06:00
 PHST- 2015/11/10 [received]
 PHST- 2016/02/17 [revised]
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 PHST- 2016/03/15 [aheadofprint]
 AID - S0045-6535(16)30241-7 [pii]
 AID - 10.1016/j.chemosphere.2016.02.081 [doi]
 PST - ppublish
 SO - Chemosphere. 2016 May;151:225-33. doi: 10.1016/j.chemosphere.2016.02.081. Epub
 2016 Mar 15.

 PMID- 27038902
 OWN - NLM
 STAT- Publisher
 DA - 20160403
 LR - 20160404
 IS - 1879-1298 (Electronic)
 IS - 0045-6535 (Linking)
 VI - 154
 DP - 2016 Mar 31
 TI - Perfluorinated alkyl acids in the plasma of South African crocodiles (*Crocodylus
 niloticus*).
 PG - 72-78
 LID - S0045-6535(16)30389-7 [pii]
 LID - 10.1016/j.chemosphere.2016.03.072 [doi]
 AB - Perfluorinated alkyl acids (PFAAs) are environmental contaminants that have been
 used in many products for over 50 years. Interest and concern has grown since
 2000 on the widespread presence of PFAAs, when it was discovered that PFAAs were

present in wildlife samples around the northern hemisphere. Since then, several studies have reported PFAAs in wildlife from many locations, including the remote regions of Antarctica and the Arctic. Although there are a multitude of studies, few have reported PFAA concentrations in reptiles and wildlife in the Southern Hemisphere. This study investigated the presence of PFAAs in the plasma of Nile crocodiles (*Crocodylus niloticus*) from South Africa. Crocodiles were captured from five sites in and around the Kruger National Park, South Africa, and plasma samples examined for PFAAs. Perfluorooctane sulfonate (PFOS) was the most frequent PFAA detected; with median values of 13.5 ng/g wet mass in crocodiles. In addition to PFOS, long chain perfluorinated carboxylic acids were also detected. Correlations between total length and PFAA load were investigated, as were differences in PFAA accumulation between sexes. No correlations were seen between crocodile size, nor were there sex-related differences. Spatial differences were examined and significant differences were observed in samples collected from the different sites ($p < 0.05$). Flag Boshielo Dam had the highest PFOS measurements, with a median concentration of 50.3 ng/g wet mass, when compared to the other sites (median concentrations at other sites below 14.0 ng/g wet mass). This suggests a point source of PFOS in this area.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20160331

TA - Chemosphere

JT - Chemosphere

JID - 0320657

OTO - NOTNLM

OT - Kruger National Park

OT - Nile crocodiles

OT - PFNA

OT - PFOS

OT - Perfluorinated alkyl acids

OT - South Africa

EDAT- 2016/04/04 06:00

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AID - 10.1016/j.chemosphere.2016.03.072 [doi]

PST - aheadofprint

SO - Chemosphere. 2016 Mar 31;154:72-78. doi: 10.1016/j.chemosphere.2016.03.072.

PMID- 26745381

OWN - NLM

STAT- In-Data-Review

DA - 20160123

IS - 1879-1298 (Electronic)

IS - 0045-6535 (Linking)
VI - 146
DP - 2016 Mar
TI - Electrochemical oxidation of perfluorinated compounds in water.
PG - 526-38
LID - 10.1016/j.chemosphere.2015.11.115 [doi]
LID - S0045-6535(15)30446-X [pii]
AB - Perfluorinated compounds (PFCs) are persistent and refractory organic pollutants that have been detected in various environmental matrices and municipal wastewater. Electrochemical oxidation (EO) is a promising remediation technique for wastewater contaminated with PFCs. A number of recent studies have demonstrated that the "non-active" anodes, including boron-doped diamond, tin oxide, and lead dioxide, are effective in PFCs elimination in wastewater due to their high oxygen evolution potential. Many researchers have conducted experiments to investigate the optimal conditions (i.e., potential, current density, pH value, plate distance, initial PFCs concentration, electrolyte, and other factors) for PFCs elimination to obtain the maximal elimination efficiency and current efficiency. The EO mechanism and pathways of PFCs have been clearly elucidated, which undergo electron transfer, Kolbe decarboxylation or desulfonation, hydrolysis, and radical reaction. In addition, the safety evaluation and energy consumption evaluation of the EO technology have also been summarized to decrease toxic ion release from electrode and reduce the cost of this technique. Although the ultrasonication and hydrothermal techniques combined with the EO process can improve the removal efficiency and current efficiency significantly, these coupled techniques have not been commercialized and applied in industrial wastewater treatment. Finally, key challenges facing EO technology are listed and the directions for further research are pointed out (such as combination with other techniques, treatment for natural waters contaminated by low levels of PFCs, and reactor design).
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 LA - eng
 PT - Journal Article
 PT - Review
 DEP - 20151230
 PL - England
 TA - Chemosphere
 JT - Chemosphere
 JID - 0320657
 SB - IM
 OTO - NOTNLM
 OT - Combination technique
 OT - Electrochemical oxidation
 OT - Electrochemical oxidation mechanisms
 OT - Energy consumption
 OT - Perfluorinated compounds
 OT - Safety evaluation
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 PMID- 27003372
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160404
 IS - 1879-1298 (Electronic)
 IS - 0045-6535 (Linking)
 VI - 152
 DP - 2016 Jun
 TI - The toxic effect and bioaccumulation in aquatic oligochaete *Limnodrilus*
hoffmeisteri after combined exposure to cadmium and perfluorooctane sulfonate at
 different pH values.
 PG - 496-502
 LID - 10.1016/j.chemosphere.2016.03.024 [doi]
 LID - S0045-6535(16)30332-0 [pii]
 AB - Cadmium (Cd) and Perfluorooctane sulfonate (PFOS) have been detected in aquatic
 environment. In this study, we investigated the acute effect, bioaccumulation and

oxidative stress status in the aquatic oligochaete *Limnodrilus hoffmeisteri* after exposure to Cd and PFOS at different pH values. In the studied pH range, acute Cd toxicity was significantly enhanced with pH increasing from 6.2 to 8.0, and the 48h-EC50 of Cd was (significantly) decreased in the presence of PFOS.

Bioaccumulation analysis results show that the accumulated Cd/PFOS in single exposure group increased with increasing exposure concentrations, and co-exposure makes internal Cd concentration significantly lowered for Cd(0.1) group at pH 8.0. Significant changes in superoxide dismutase activity, glutathione level and malondialdehyde content were observed in single and combined treatments. Based on IBR value, single Cd and PFOS exposure caused largest damage to the antioxidant defense system at pH 8.0 and pH 6.2, respectively, while the harmful effects of joint exposure were always the "compromise" between single Cd and PFOS exposure. This work could provide useful information for the risk assessment of co-exposure to perfluorinated compounds and heavy metals in natural environment.

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LA - eng

PT - Journal Article

DEP - 20160319

PL - England

TA - Chemosphere

JT - Chemosphere

JID - 0320657

SB - IM

OTO - NOTNLM

OT - Acute toxicity

OT - Bioaccumulation

OT - Cadmium

OT - Oxidative stress

OT - Perfluorooctane sulfonate

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AID - S0045-6535(16)30332-0 [pii]
AID - 10.1016/j.chemosphere.2016.03.024 [doi]
PST - ppublish
SO - Chemosphere. 2016 Jun;152:496-502. doi: 10.1016/j.chemosphere.2016.03.024. Epub 2016 Mar 19.

PMID- 26991379
OWN - NLM
STAT- In-Data-Review
DA - 20160404
IS - 1879-1298 (Electronic)
IS - 0045-6535 (Linking)
VI - 152
DP - 2016 Jun
TI - Uptake of 8:2 perfluoroalkyl phosphate diester and its degradation products by carrot and lettuce from compost-amended soil.
PG - 309-17
LID - 10.1016/j.chemosphere.2016.02.130 [doi]
LID - S0045-6535(16)30303-4 [pii]
AB - The present work studied the uptake of 8:2 perfluoroalkyl phosphate diester (diPAP) by two different crops (lettuce and carrot) and two different amended soils. Firstly, the possible degradation of 8:2 diPAP in the absence of crop was studied and 8:2 monoPAP (monophosphate), 8:2 FTCA (saturated fluorotelomer carboxylate), 8:2 FTUCA (unsaturated fluorotelomer carboxylate), 7:3 FTCA (saturated fluorotelomer carboxylate), PFHpA (perfluoroheptanoic acid), PFHxA (perfluorohexanoic acid) and PFOA (perfluorooctanoic acid) were detected. In the presence of crops, different degradation products were detected in the soil and, while PFNA (perfluorononanoic acid), PFHpA, PFHxA, PFPeA (perfluoropentanoic acid), PFBA (perfluorobutanoic acid), 7:3 FTCA and PFOA were determined in the cultivation media when carrot was grown, PFOA was the only degradation product detected in the case of lettuce experiments. Regarding the uptake in carrot, all the degradation products except 7:3 FTCA were translocated from the soil to the carrot. Carrot core, peel and leaves bioconcentration factors, BCFs, were determined for 8:2 diPAP and its degradation products. Values lower than method detection limits for core and low BCFs in peel (0.025-0.042) and leaves (0.028-0.049) were achieved for 8:2 diPAP. Regarding to the degradation products, the higher their water solubility, the higher the plant translocation. In this sense, the lower the carbon chain length of PFCAs, the higher the BCFs determined (PFBA > PFHxA > PFHpA > PFOA > PFNA). In general, lower total BCFs were achieved when the total organic carbon of the soils increased. For lettuce experiments, 8:2 diPAP (0.04-0.18) and PFOA (0.28-1.57) were only determined in lettuce heart.
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LA - eng
PT - Journal Article
DEP - 20160315
PL - England
TA - Chemosphere
JT - Chemosphere
JID - 0320657
SB - IM
OTO - NOTNLM
OT - 8:2 diPAP
OT - Amended soil
OT - Bioconcentration factor
OT - Crops
OT - PFOA
EDAT- 2016/03/19 06:00
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SO - Chemosphere. 2016 Jun;152:309-17. doi: 10.1016/j.chemosphere.2016.02.130. Epub 2016 Mar 15.

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OWN - NLM
STAT- Publisher
DA - 20160319
LR - 20160320
IS - 1520-636X (Electronic)
IS - 0899-0042 (Linking)
DP - 2016 Mar 18
TI - Helical Inversion of Gel Fibrils by Elongation of Perfluoroalkyl Chains as Studied by Vibrational Circular Dichroism.
LID - 10.1002/chir.22592 [doi]
AB - Vibrational circular dichroism (VCD) spectroscopy was applied to gelation by a chiral low-molecular mass weight gelator, N,N'-diperfluoroalkanoyl-1,2-trans-diaminocyclohexane. Attention was focused on the winding effects of $(-CF_2)_n$ chains on the gelating ability. For this purpose, a series of gelators were synthesized with perfluoroalkyl chains of different length ($n = 6-8$). When gelation was studied using acetonitrile as a solvent, the fibrils took different morphologies, depending on the chain length: twisted saddle-like ribbon or helical ribbon from fibril ($n = 6$) and a helical ribbon from platelet ($n = 8$). The signs of VCD peaks assigned to the couplet of C=O stretching and to the C-F stretching were also dependent on n , indicating that a gelator molecule changed conformation on elongating perfluoroalkyl chains. A model is proposed for the aggregation modes in fibrils. Chirality 00:000-000, 2016. (c) 2016 Wiley Periodicals, Inc.
CI - (c) 2016 Wiley Periodicals, Inc.
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LA - ENG
PT - JOURNAL ARTICLE
DEP - 20160318
TA - Chirality
JT - Chirality
JID - 8914261
OTO - NOTNLM
OT - chiral gelator
OT - perfluoroalkyl chains
OT - supramolecular
OT - vibrational circular dichroism
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 AID - 10.1002/chir.22592 [doi]
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PMID- 26942927
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160407
 IS - 1573-3017 (Electronic)
 IS - 0963-9292 (Linking)
 VI - 25
 IP - 4
 DP - 2016 May
 TI - Gene expression profile changes in *Eisenia fetida* chronically exposed to PFOA.
 PG - 759-69
 LID - 10.1007/s10646-016-1634-x [doi]
 AB - *Eisenia fetida* is a terrestrial organism, which can be used to diagnose sub-lethal concentrations of PFOA by using molecular biomarkers. In order to identify potential molecular biomarkers, we have exposed *E. fetida* to 10 mg/kg of PFOA in soil for 8 months. The mRNA isolation, sequencing, transcriptome assembly followed by differential gene expression studies have revealed that genes that are involved in apoptotic process, reproduction, calcium signalling, neuronal development and lipid metabolism are predominantly affected. Highly specific genes that are altered by PFOA can be further validated and used as biomarker to detect sub-lethal concentrations of PFOA in the soil.

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 LA - eng
 PT - Journal Article
 DEP - 20160304
 PL - United States
 TA - Ecotoxicology
 JT - Ecotoxicology (London, England)
 JID - 9885956
 SB - IM
 OTO - NOTNLM
 OT - Differential gene expression
 OT - Eisenia fetida
 OT - Perfluorooctanoic acid (PFOA)
 OT - Toxicogenomics
 OT - Transcriptome assembly
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 AID - 10.1007/s10646-016-1634-x [pii]
 PST - ppublish
 SO - Ecotoxicology. 2016 May;25(4):759-69. doi: 10.1007/s10646-016-1634-x. Epub 2016 Mar 4.

 PMID- 26978841
 OWN - NLM
 STAT- Publisher
 DA - 20160315
 LR - 20160316
 IS - 1552-9924 (Electronic)
 IS - 0091-6765 (Linking)
 DP - 2016 Mar 15
 TI - Modeled Perfluorooctanoic Acid (PFOA) Exposure and Liver Function in a Mid-Ohio Valley Community.
 AB - BACKGROUND: Perfluorooctanoic acid (PFOA or C8) has hepatotoxic effects in animals. Cross-sectional epidemiologic studies suggest PFOA is associated with liver injury biomarkers. OBJECTIVES: We estimated associations between modeled historical PFOA exposures and liver injury biomarkers and medically-validated liver disease. METHODS: Participants completed surveys during 2008-2011 reporting demographic, medical, and residential history information. Self-reported liver disease, including hepatitis, fatty liver, enlarged liver and cirrhosis, was validated with healthcare providers. Alanine aminotransferase (ALT),

gamma-glutamyltransferase (GGT) and direct bilirubin, markers of liver toxicity, were obtained from blood samples collected in the C8 Health Project (2005-2006). Historically modeled PFOA exposure, estimated using environmental fate and transport models and participant residential histories, was analyzed in relation to liver biomarkers (n=30,723, including 1892 workers) and liver disease (n=32,254, including 3713 workers). RESULTS: Modeled cumulative serum PFOA was positively associated with ALT levels (p for trend <0.0001), indicating possible liver toxicity. An increase from the first to the fifth quintile of cumulative PFOA exposure was associated with a 6% increase in ALT levels (95%CI: 4-8%) and a 16% increased odds of having above-normal ALT (95%CI odds ratio: 1.02-1.33%). There was no indication of association with either elevated direct bilirubin or GGT; however, PFOA was associated with decreased direct bilirubin. We observed no evidence of an effect of cumulative exposure (with or without a 10-year lag) on all liver disease (n=647 cases), nor on enlarged liver, fatty liver and cirrhosis only (n=427 cases). CONCLUSION: Results are consistent with previous cross-sectional studies showing association between PFOA and ALT, a marker of hepatocellular damage. We did not observe evidence that PFOA increases the risk of clinically-diagnosed liver disease.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20160315

TA - Environ Health Perspect
 JT - Environmental health perspectives
 JID - 0330411
 EDAT- 2016/03/16 06:00
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 AID - 10.1289/ehp.1510391 [doi]
 AID - ehp.1510391 [pii]
 PST - aheadofprint
 SO - Environ Health Perspect. 2016 Mar 15.

PMID- 26115335
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160302
 LR - 20160317
 IS - 1552-9924 (Electronic)
 IS - 0091-6765 (Linking)
 VI - 124
 IP - 3
 DP - 2016 Mar
 TI - Prenatal Phthalate, Perfluoroalkyl Acid, and Organochlorine Exposures and Term Birth Weight in Three Birth Cohorts: Multi-Pollutant Models Based on Elastic Net Regression.
 PG - 365-72
 LID - 10.1289/ehp.1408933 [doi]
 AB - BACKGROUND: Some legacy and emerging environmental contaminants are suspected risk factors for intrauterine growth restriction. However, the evidence is equivocal, in part due to difficulties in disentangling the effects of mixtures. OBJECTIVES: We assessed associations between multiple correlated biomarkers of environmental exposure and birth weight. METHODS: We evaluated a cohort of 1,250 term (≥ 37 weeks gestation) singleton infants, born to 513 mothers from Greenland, 180 from Poland, and 557 from Ukraine, who were recruited during antenatal care visits in 2002-2004. Secondary metabolites of diethylhexyl and diisononyl phthalates (DEHP, DiNP), eight perfluoroalkyl acids, and organochlorines (PCB-153 and p,p -DDE) were quantifiable in 72/100% of maternal serum samples. We assessed associations between exposures and term birth weight, adjusting for co-exposures and covariates, including prepregnancy body mass index. To identify independent associations, we applied the elastic net penalty to linear regression models. RESULTS: Two phthalate metabolites (MEHHP, MOiNP), perfluorooctanoic acid (PFOA), and p,p -DDE were most consistently predictive of term birth weight based on elastic net penalty regression. In an adjusted, unpenalized regression model of the four exposures, 2-SD increases in natural log-transformed MEHHP, PFOA, and p,p -DDE were associated with lower birth weight: -87 g (95% CI: -137, -340 per 1.70 ng/mL), -43 g (95% CI: -108, 23 per

1.18 ng/mL), and -135 g (95% CI: -192, -78 per 1.82 ng/g lipid), respectively; and MOiNP was associated with higher birth weight (46 g; 95% CI: -5, 97 per 2.22 ng/mL). CONCLUSIONS: This study suggests that several of the environmental contaminants, belonging to three chemical classes, may be independently associated with impaired fetal growth. These results warrant follow-up in other cohorts. CITATION: Lenters V, Portengen L, Rignell-Hydbom A, Jonsson BA, Lindh CH, Piersma AH, Toft G, Bonde JP, Heederik D, Rylander L, Vermeulen R. 2016. Prenatal phthalate, perfluoroalkyl acid, and organochlorine exposures and term birth weight in three birth cohorts: multi-pollutant models based on elastic net regression. Environ Health Perspect 124:365-372; <http://dx.doi.org/10.1289/ehp.1408933>.

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FAU - Vermeulen, Roel

AU - Vermeulen R

LA - eng

PT - Journal Article

DEP - 20150626

PL - United States

TA - Environ Health Perspect

JT - Environmental health perspectives

JID - 0330411

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PMC - PMC4786980

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OWN - NLM
STAT- In-Data-Review
DA - 20160411
IS - 1873-6750 (Electronic)
IS - 0160-4120 (Linking)
VI - 91
DP - 2016 May
TI - Perfluoroalkyl substances in older male anglers in Wisconsin.
PG - 312-8
LID - 10.1016/j.envint.2016.03.012 [doi]
LID - S0160-4120(16)30092-7 [pii]
AB - BACKGROUND: Perfluoroalkyl substances (PFAS) are an emerging class of contaminants. Certain PFAS are regulated or voluntarily limited due to concern about environmental persistence and adverse health effects, including thyroid disease and to dyslipidemia. The major source of PFAS exposure in the general population is seafood. OBJECTIVES: In this analysis we examine PFAS levels and their determinants, as well as associations between PFAS levels and self-reported health outcomes, in a group of older male anglers in Wisconsin with high fish consumption. METHODS: A biomonitoring study of male anglers aged 50 and older living in Wisconsin collected detailed information on fish consumption, demographics and self-reported health outcomes, along with hair and blood samples for biomarker analysis. Sixteen different PFAS were extracted from serum samples. Regression models were used to identify factors (demographic characteristics and fish consumption habits) associated with PFAS biomarker levels in blood, as well as associations between PFAS and self-reported health outcomes, adjusting for potential confounders. RESULTS: Seven PFAS were detected in at least 30% of participants and were used in subsequent analyses (PFDA, PFHpS, PFHxS, PFNA, PFOA, PFOS, PFuDA). The PFAS with the highest levels were PFOS, followed by PFOA, PFHxS and PFNA (medians of 19.0, 2.5, 1.8 and 1.4ng/mL). In general, increasing age was associated with higher PFAS levels, while increasing BMI were associated with lower PFAS levels. Greater alcohol consumption was associated with higher levels of PFHpS, PFHxS and PFOA. Associations with smoking and employment did not show a consistent pattern. Associations between fish consumption and PFAS were generally weak, with the exception of notably higher PFDA and PFHpS with both other locally-caught fish, and restaurant-purchased fish. Regarding associations with health outcomes, PFuDA, PFNA and PFDA were all associated with increased risk of pre-diabetes and/or diabetes. PFHpS was associated with a significantly increased risk of high cholesterol; PFDA and PFuDA also showed notable, though non-significant associations. All PFAS evaluated were associated with lower risk

of hypertension although the only significant odds ratio was that for PFNA. There were no associations between any of the PFAS examined and either coronary heart disease, or the grouped outcome of any cardiovascular condition. CONCLUSIONS: PFAS are emerging contaminants with widespread exposure, persistence, and potential for adverse health effects. In this study population, demographic patterns may reflect differences in exposure sources, or possibly differences in adsorption and metabolism. PFAS were associated mainly with endocrine related outcomes, with a general trend towards increased risk of glucose intolerance and high cholesterol. Continued research on the risks and benefits of fish consumption is important due to potential exposure to PFAS and noted associations with highly prevalent adverse health outcomes.

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LA - eng

PT - Journal Article

DEP - 20160319

PL - Netherlands

TA - Environ Int

JT - Environment international

JID - 7807270

SB - IM

OTO - NOTNLM

OT - Angler

OT - Contaminant

OT - Environmental exposure

OT - PFAS

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OWN - NLM
STAT- In-Data-Review
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IS - 1873-6750 (Electronic)
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VI - 91
DP - 2016 May
TI - Properties, performance and associated hazards of state-of-the-art durable water repellent (DWR) chemistry for textile finishing.
PG - 251-64
LID - 10.1016/j.envint.2016.02.035 [doi]
LID - S0160-4120(16)30071-X [pii]
AB - Following the phase-out of long-chain per- and polyfluoroalkyl substances (PFASs), the textile industry had to find alternatives for side-chain fluorinated polymer based durable water repellent (DWR) chemistries that incorporated long perfluoroalkyl side chains. This phase-out and subsequent substitution with alternatives has resulted in a market where both fluorinated and non-fluorinated DWRs are available. These DWR alternatives can be divided into four broad groups that reflect their basic chemistry: side-chain fluorinated polymers, silicones, hydrocarbons and other chemistries (includes dendrimer and inorganic nanoparticle chemistries). In this critical review, the alternative DWRs are assessed with regards to their structural properties and connected performance, loss and degradation processes resulting in diffuse environmental emissions, and hazard profiles for selected emitted substances. Our review shows that there are large differences in performance between the alternative DWRs, most importantly the lack of oil repellence of non-fluorinated alternatives. It also shows that for all alternatives, impurities and/or degradation products of the DWR chemistries are diffusively emitted to the environment. Our hazard ranking suggests that hydrocarbon based DWR is the most environmentally benign, followed by silicone and side-chain fluorinated polymer-based DWR chemistries. Industrial commitments to reduce the levels of impurities in silicone based and side-chain fluorinated polymer based DWR formulations will lower the actual risks. There is a lack of information on the hazards associated with DWRs, in particular for the dendrimer and inorganic nanoparticle chemistries, and these data gaps must be filled. Until environmentally safe alternatives, which provide the required performance, are available our recommendation is to choose DWR chemistry on a case-by-case basis, always weighing the benefits connected to increased performance against the risks to the environment and human health.

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LA - eng

PT - Journal Article

PT - Review

DEP - 20160316

PL - Netherlands

TA - Environ Int

JT - Environment international

JID - 7807270

SB - IM

OTO - NOTNLM

OT - Dendrimers

OT - Hazard assessment

OT - PFAS

OT - Per- and polyfluoroalkyl substances

OT - Silicones

OT - Wax

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SO - Environ Int. 2016 May;91:251-64. doi: 10.1016/j.envint.2016.02.035. Epub 2016 Mar 16.

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OWN - NLM

STAT- In-Data-Review

DA - 20160215

IS - 1873-6750 (Electronic)

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VI - 88

DP - 2016 Mar

TI - Perfluoroalkyl substances and food allergies in adolescents.

PG - 74-9

LID - 10.1016/j.envint.2015.12.020 [doi]

LID - S0160-4120(15)30122-7 [pii]

AB - Perfluoroalkyl and polyfluoroalkyl substances (PFASs) are a class of organic compounds that are persistent in the environment due to their stable carbon-fluorine backbone, which is not susceptible to degradation. Research suggests these chemicals may exert an immunotoxic effect. The aim of this study is to investigate the associations between four PFASs - perfluorooctane sulfonic acid (PFOS), perfluorooctanoic acid (PFOA), perfluorononanoic acid (PFNA), and perfluorohexane sulfonic acid (PFHxS) - with food sensitization and food allergies in adolescent participants (ages 12-19years) in the National Health and Nutrition Examination Survey (NHANES) 2005-2006 and 2007-2010, respectively. We performed multivariate logistic regression to analyze the association between individual PFASs with food sensitization (defined as having at least 1 food-specific IgE level ≥ 0.35 kU/L) in NHANES 2005-2006 and food allergies (self-reported) in NHANES 2007-2010. Serum PFOA, PFOS, and PFHxS were statistically significantly associated with higher odds to have self-reported food allergies in NHANES 2007-2010. When using IgE levels as a marker of food sensitization, we found that serum PFNA was inversely associated with food sensitization (NHANES 2005-2006). In conclusion, we found that serum levels of PFASs were associated with higher odds to have self-reported food allergies. Conversely, adolescents with higher serum PFNA were less likely to be sensitized to food allergens. These results, along with previous studies, warrant further investigation, such as well-designed longitudinal studies.

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LA - eng

PT - Journal Article
 DEP - 20151223
 PL - Netherlands
 TA - Environ Int
 JT - Environment international
 JID - 7807270
 SB - IM
 OTO - NOTNLM
 OT - Adolescents
 OT - Food allergies
 OT - NHANES
 OT - Perfluoroalkyl compounds
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 OWN - NLM
 STAT- In-Data-Review
 DA - 20160215
 IS - 1873-6750 (Electronic)
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 VI - 88
 DP - 2016 Mar
 TI - Serum perfluorinated chemicals, glucose homeostasis and the risk of diabetes in working-aged Taiwanese adults.
 PG - 15-22
 LID - 10.1016/j.envint.2015.11.016 [doi]
 LID - S0160-4120(15)30100-8 [pii]
 AB - BACKGROUND: The link among perfluoroalkyl and polyfluoroalkyl substances (PFASs), abnormal glucose homeostasis and the risk of diabetes has been intensively debated with conflicting evidence. OBJECTIVES: We evaluated the associations among PFASs, oral glucose tolerance testing (OGTT) curves and diabetes prevalence in 571 working-aged Taiwanese participants. METHODS: Exposure measures included serum perfluorooctanoic acid (PFOA), perfluorooctane sulfonic acid (PFOS), perfluorononanoic acid (PFNA), and perfluoroundecanoic acid (PFUA). Outcomes were OGTT curves and prevalent diabetes defined by fasting blood glucose (FBG) ≥ 126 mg/dL, 2-h glucose ≥ 200 mg/dL, or glycated hemoglobin $\geq 6.5\%$. Analyses were performed with multiple logistic regression and functional data analysis.

RESULTS: A total of 39 participants (6.8%) had diabetes in this study. After full adjustment, the increase in the geometric means of FBG, 2-h glucose concentrations, and area under the OGTT curve (AUC₁₂₀) with a doubling increase in PFOS was 3% (95% CI 1-4), 8% (5-12), and 6% (4-9), respectively. Compared to the lowest-quartile of PFOS concentrations (<2.4ng/ml), the OGTT trajectories were significantly steeper in participants of the highest-quartile PFOS exposure (>4.8ng/ml) and the vertical shifting of the mean curve for each PFOS quartile showed a dose-response pattern. The adjusted odds ratio for diabetes comparing the highest to lowest quartile was 3.37 (95% CI 1.18-9.65). For PFOA, PFNA, and PFUA, the opposite pattern of OGTT trajectory and the opposite risk profile for diabetes were observed. CONCLUSIONS: Chronic PFOS exposure was associated with impaired glucose homeostasis and the increased prevalence of diabetes. However, PFOA, PFNA, and PFUA showed a potential protective effect against glucose intolerance and the risk of diabetes. Future research focusing on clarifying possible differential effects of different species of PFASs on glucose homeostasis and establishing the prospective associations between PFASs and diabetes is needed.

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LA - eng

PT - Journal Article

DEP - 20151214

PL - Netherlands

TA - Environ Int

JT - Environment international

JID - 7807270

SB - IM

OTO - NOTNLM

OT - Diabetes

OT - Glucose homeostasis

OT - Oral glucose tolerance testing

OT - Perfluorinated chemicals

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LR - 20160310

IS - 1873-6424 (Electronic)

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TI - Neutral and ionic per- and polyfluoroalkyl substances (PFASs) in atmospheric and dry deposition samples over a source region (Tianjin, China).

PG - 449-456

LID - S0269-7491(16)30128-2 [pii]

LID - 10.1016/j.envpol.2016.02.023 [doi]

AB - Per- and polyfluoroalkyl substances (PFASs) were detected in the atmosphere of a source region in Tianjin, China. Fluorotelomer alcohols (FTOHs) were the dominant neutral PFASs in the atmosphere with total concentrations of 93.6-131 pg/m3 and 8:2 FTOH contributing the most, whereas perfluorooctane sulfonamide derivatives (PFOSAs) were two magnitudes lower or undetected. In comparison, ionic PFASs

(perfluoroalkyl carboxyl acids (PFCAs)) in the atmosphere were detected at similar or even higher levels. At wastewater treatment plants (WWTPs), the air over influent was found with higher levels of FTOHs than over aeration tank and effluent; whereas in the air over the aeration tank, the concentrations of PFOSAs and nonvolatile ionic PFASs substantially increased, suggesting a possible direct release of ionic PFASs to the atmosphere besides the atmospheric conversion from volatile precursors. In the air phase, a low proportion (1–5%) of PFCAs was subjected to dry deposition in the source region. Interestingly, the dry-deposition-to-bulk-air ratios of PFCA analogues were the lowest at medium chain lengths (C8 and C9) and increased with either shorter or longer chain length. The extraordinary affinity of shorter-chain PFCAs (C6–C7) to particles was presumed to be due to their smaller molecular size favoring the interactions between the carboxyl head groups and specific sorption sites on particulate matter.

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LA - ENG
PT - JOURNAL ARTICLE
DEP - 20160304
TA - Environ Pollut
JT - Environmental pollution (Barking, Essex : 1987)
JID - 8804476
OTO - NOTNLM
OT - Atmosphere
OT - Dry deposition
OT - Long range transport
OT - Per- and polyfluoroalkyl substances
OT - Wastewater treatment plant
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AID - 10.1016/j.envpol.2016.02.023 [doi]
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PMID- 26970855
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VI - 212
DP - 2016 Mar 10
TI - Positive associations of serum perfluoroalkyl substances with uric acid and
hyperuricemia in children from Taiwan.
PG - 519-524
LID - S0269-7491(16)30176-2 [pii]
LID - 10.1016/j.envpol.2016.02.050 [doi]
AB - To investigate the risk of hyperuricemia in relation to Perfluoroalkyl substances
(PFASs) in children from Taiwan, 225 Taiwanese children aged 12-15 years were
recruited from 2009 to 2010. Linear and logistic regression models were employed
to examine the influence of PFASs on serum uric acid levels. Findings revealed
that eight of ten PFASs analyses were detected in >94% of the participants' serum
samples. Multivariate linear regression models revealed that perfluorooctanoic
acid (PFOA) was positively associated with serum uric acid levels (beta = 0.1463,
p < 0.05). Of all the PFASs analyses, only PFOA showed a significant effect on
elevated levels of hyperuricemia (aOR = 2.16, 95%CI: 1.29-3.61). When stratified

by gender, the association between serum PFOA and uric acid levels was only evident among boys (aOR = 2.76, 95%CI: 1.37-5.56). In conclusion, PFOA was found to be associated with elevated serum levels of uric acid in Taiwanese children, especially boys. Further research is needed to elucidate these links.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20160310

TA - Environ Pollut

JT - Environmental pollution (Barking, Essex : 1987)

JID - 8804476

OTO - NOTNLM

OT - Children

OT - Hyperuricemia
 OT - Perfluoroalkyl substances
 OT - Uric acid
 EDAT- 2016/03/14 06:00
 MHDA- 2016/03/14 06:00
 CRDT- 2016/03/14 06:00
 PHST- 2016/01/15 [received]
 PHST- 2016/02/24 [revised]
 PHST- 2016/02/24 [accepted]
 AID - S0269-7491(16)30176-2 [pii]
 AID - 10.1016/j.envpol.2016.02.050 [doi]
 PST - aheadofprint
 SO - Environ Pollut. 2016 Mar 10;212:519-524. doi: 10.1016/j.envpol.2016.02.050.

PMID- 26974364
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160404
 IS - 1096-0953 (Electronic)
 IS - 0013-9351 (Linking)
 VI - 147
 DP - 2016 May
 TI - Analysis of the presence of perfluoroalkyl substances in water, sediment and biota of the Jucar River (E Spain). Sources, partitioning and relationships with water physical characteristics.
 PG - 503-12
 LID - 10.1016/j.envres.2016.03.010 [doi]
 LID - S0013-9351(16)30090-1 [pii]
 AB - The presence, sources and partitioning of 21 perfluoroalkyl substances (PFASs: C4-C14, C16, C18 carboxylate, C4, C6-C10 sulfonates and C8 sulfonamide) were assessed in water, sediment, and biota of the Jucar River basin (E Spain). Considering the three matrices, perfluoropentanoate (PFPeA) and perfluorooctane sulfonate (PFOS) were the most frequent compounds, being remarkable the high occurrence of short-chain PFASs ($C \leq 8$), which are intended to replace the long-chain ones in several industrial and commercial applications. In general, all samples were contaminated with at least one PFAS, with the exception of three fish samples. Mean concentrations detected in sediments ($0.22-11.5 \text{ ng g}^{-1}$) and biota ($0.63-274 \text{ microg kg}^{-1}$) samples were higher than those measured in water ($0.04-83.1 \text{ ng L}^{-1}$), which might suggest (bio) accumulation. The occurrence of PFAS is related to urban and industrial discharges (Cuenca city in the upper part of basin, and car's factory, and effluents of the sewage treatment plant (STP) of Alzira, in the lower part). Increasing pollution gradients were found. On the other hand, higher contamination levels were observed after regulation dams of the catchment pointing out their importance in the re-distribution of these contaminants. None of the hazard quotients (HQ) calculated indicate potential risk for the different trophic levels considered (algae, *Daphnia* sp. and fish). PFAS concentrations found in this study can be considered in acceptable levels if compared to existing Regulatory Legislation and, consequently, they do not pose

an immediate human health risk.

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LA - eng

PT - Journal Article

DEP - 20160311

PL - United States

TA - Environ Res

JT - Environmental research

JID - 0147621

SB - IM

OTO - NOTNLM

OT - Bioaccumulation

OT - Hazard quotient

OT - LC-MS/MS

OT - Mediterranean ecosystem

OT - Perfluoroalkyl substances

OT - Regulation dam
 EDAT- 2016/03/15 06:00
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 PHST- 2016/03/11 [aheadofprint]
 AID - S0013-9351(16)30090-1 [pii]
 AID - 10.1016/j.envres.2016.03.010 [doi]
 PST - ppublish
 SO - Environ Res. 2016 May;147:503-12. doi: 10.1016/j.envres.2016.03.010. Epub 2016 Mar 11.

 PMID- 26950028
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160404
 IS - 1096-0953 (Electronic)
 IS - 0013-9351 (Linking)
 VI - 147
 DP - 2016 May
 TI - Perfluoroalkyl substances in serum from South Korean infants with congenital hypothyroidism and healthy infants - Its relationship with thyroid hormones.
 PG - 399-404
 LID - 10.1016/j.envres.2016.02.037 [doi]
 LID - S0013-9351(16)30078-0 [pii]
 AB - Exposure to perfluoroalkyl substances (PFASs) may disrupt thyroid systems, though the specific effects of PFASs are still being elucidated. Since research regarding exposure in infants is highly limited, our goal was to investigate exposure levels of PFASs in infant serum and correlate these levels with thyroid hormones (THs). This was accomplished by analyzing 16 PFASs in sera from a case group of infants with congenital hypothyroidism and a control group. Total PFAS exposure level was 2.63-44.7ng/mL in the case group and 2.44-22.4ng/mL in the control group. Concentrations of serum perfluorooctanoic acid (PFOA, $p<0.01$), perfluorononanoic acid (PFNA, $p<0.001$), perfluorooctanoic acid (PFDA, $p<0.005$), and perfluoroundecanoic acid (PFUnDA, $p<0.005$) were significantly higher in the case group than the control group. Levels of certain PFASs (PFOA, perfluorotridecanoic acid [PFTrDA], and perfluorohexane sulfonate [PFHxS]) showed a moderate to weak correlation with relevant antibodies.
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 LA - eng
 PT - Journal Article
 DEP - 20160304
 PL - United States
 TA - Environ Res
 JT - Environmental research
 JID - 0147621
 SB - IM
 OTO - NOTNLM
 OT - Congenital hypothyroidism
 OT - Infant
 OT - Perfluoroalkyl substances
 OT - Serum
 OT - South Korea
 EDAT- 2016/03/08 06:00
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 PHST- 2016/03/04 [aheadofprint]
 AID - S0013-9351(16)30078-0 [pii]
 AID - 10.1016/j.envres.2016.02.037 [doi]
 PST - ppublish
 SO - Environ Res. 2016 May;147:399-404. doi: 10.1016/j.envres.2016.02.037. Epub 2016
 Mar 4.

 PMID- 27030239
 OWN - NLM
 STAT- Publisher
 DA - 20160331
 LR - 20160401
 IS - 1614-7499 (Electronic)
 IS - 0944-1344 (Linking)
 DP - 2016 Mar 31

TI - Photochemical defluorination of aqueous perfluorooctanoic acid (PFOA) by Fe/GAC micro-electrolysis and VUV-Fenton photolysis.

AB - Perfluorooctanoic acid (PFOA) is extremely persistent and bioaccumulative in the environment; thus, it is very urgent to investigate an effective and moderate technology to treat the pollution of PFOA. In this study, a process combined iron and granular activated carbon (Fe0/GAC) micro-electrolysis with VUV-Fenton system is employed for the remediation of PFOA. Approximately 50 % PFOA (10 mg L⁻¹) could be efficiently defluorinated under the following conditions: pH 3.0, dosage of Fe 7.5 g L⁻¹, dosage of GAC 12.5 g L⁻¹, and concentration of H₂O₂ 22.8 mmol L⁻¹. Meanwhile, during the process, evident defluorination was observed and the concentration of fluoride ion was eventually 3.23 mg L⁻¹. The intermediates including five shorter-chain perfluorinated carboxylic acids (PFCAs), i.e., C₇, C₆, C₅, C₄, and C₃, were also analyzed by high-performance liquid chromatography tandem mass spectrometry (HPLC/MS/MS) and defluorination mechanisms of PFOA was proposed, which involved photochemical of OH[·], direct photolysis (185-nm VUV), and photocatalytic degradation of PFOA in the presence of Fe³⁺ (254-nm UV).

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20160331
 TA - Environ Sci Pollut Res Int
 JT - Environmental science and pollution research international
 JID - 9441769
 OTO - NOTNLM
 OT - Defluorination
 OT - Fe⁰/GAC micro-electrolysis
 OT - Intermediates
 OT - Mechanisms
 OT - PFOA
 OT - VUV-Fenton
 EDAT- 2016/04/01 06:00
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 PHST- 2015/12/03 [received]
 PHST- 2016/03/21 [accepted]
 PHST- 2016/03/31 [aheadofprint]
 AID - 10.1007/s11356-016-6539-y [doi]
 AID - 10.1007/s11356-016-6539-y [pii]
 PST - aheadofprint
 SO - Environ Sci Pollut Res Int. 2016 Mar 31.

 PMID- 26585456
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160403
 IS - 1614-7499 (Electronic)
 IS - 0944-1344 (Linking)
 VI - 23
 IP - 6
 DP - 2016 Mar
 TI - Depth profile of persistent and emerging organic pollutants upstream of the Three Gorges Dam gathered in 2012/2013.
 PG - 5782-94
 LID - 10.1007/s11356-015-5805-8 [doi]
 AB - Persistent and emerging organic pollutants were sampled in September 2012 and 2013 at a sampling site in front of the Three Gorges Dam near Maoping (China) in a water depth between 11 and 61 m to generate a depth profile of analytes. A novel compact water sampling system with self-packed glass cartridges was employed for the on-site enrichment of approximately 300 L of water per sample to enable the detection of low analytes levels in the picogram per liter-scale in the large water body. The overall performance of the sampling system was acceptable for the qualitative detection of polycyclic aromatic hydrocarbons (PAHs), polychlorinated biphenyls (PCBs), organochlorine pesticides (OCPs), perfluoroalkyl acids (PFAAs), pharmaceutical residues and polar pesticides. Strongly particle-associated analytes like PAHs and PCBs resided mainly in the glass wool filter of the sampling system, whereas all other compounds have mainly been enriched on the XAD-resin of the self-packed glass cartridges. The sampling

results revealed qualitative information on the presence, depth distribution and origin of the investigated compounds. Although the depth profile of PAHs, PCBs, OCPs, and PFAAs appeared to be homogeneous, pharmaceuticals and polar pesticides were detected in distinct different patterns with water depth. Source analysis with diagnostic ratios for PAHs revealed their origin to be pyrogenic (burning of coal, wood and grass). In contrast, most PCBs and OCPs had to be regarded as legacy pollutants which have been released into the environment in former times and still remain present due to their persistence. The abundance of emerging organic pollutants could be confirmed, and their most abundant compounds could be identified as perfluorooctanoic acid, diclofenac and atrazine among investigated PFAAs, pharmaceuticals and polar pesticides, respectively.

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LA - eng
PT - Journal Article
DEP - 20151120
PL - Germany
TA - Environ Sci Pollut Res Int
JT - Environmental science and pollution research international
JID - 9441769
SB - IM
OTO - NOTNLM
OT - Depth profile
OT - Environmental fate
OT - Monitoring
OT - Perfluoroalkylic acids
OT - Persistent organic compounds
OT - Pharmaceutical residues
EDAT- 2015/11/21 06:00
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PHST- 2015/07/28 [received]
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PHST- 2015/11/20 [aheadofprint]
AID - 10.1007/s11356-015-5805-8 [doi]
AID - 10.1007/s11356-015-5805-8 [pii]
PST - ppublish
SO - Environ Sci Pollut Res Int. 2016 Mar;23(6):5782-94. doi:
10.1007/s11356-015-5805-8. Epub 2015 Nov 20.

PMID- 26866280
OWN - NLM
STAT- In-Data-Review
DA - 20160301
IS - 1520-5851 (Electronic)
IS - 0013-936X (Linking)
VI - 50
IP - 5
DP - 2016 Mar 1
TI - Influence of Perfluorooctanoic Acid on the Transport and Deposition Behaviors of
Bacteria in Quartz Sand.
PG - 2381-8
LID - 10.1021/acs.est.5b05496 [doi]
AB - The significance of perfluorooctanoic acid (PFOA) on the transport and deposition
behaviors of bacteria (Gram-negative Escherichia coli and Gram-positive Bacillus
subtilis) in quartz sand is examined in both NaCl and CaCl₂ solutions at pH 5.6
by comparing both breakthrough curves and retained profiles with PFOA in
solutions versus those without PFOA. All test conditions are found to be highly
unfavorable for cell deposition regardless of the presence of PFOA; however,
7%-46% cell deposition is observed depending on the conditions. The cell

deposition may be attributed to micro- or nanoscale roughness and/or to chemical heterogeneity of the sand surface. The results show that, under all examined conditions, PFOA in suspensions increases cell transport and decreases cell deposition in porous media regardless of cell type, presence or absence of extracellular polymeric substances, ionic strength, and ion valence. We find that the additional repulsion between bacteria and quartz sand caused by both acid-base interaction and steric repulsion as well as the competition for deposition sites on quartz sand surfaces by PFOA are responsible for the enhanced transport and decreased deposition of bacteria with PFOA in solutions.

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LA - eng

PT - Journal Article

DEP - 20160219

PL - United States

TA - Environ Sci Technol

JT - Environmental science & technology

JID - 0213155

SB - IM

EDAT- 2016/02/13 06:00

MHDA- 2016/02/13 06:00

CRDT- 2016/02/12 06:00

PHST- 2016/02/19 [aheadofprint]

AID - 10.1021/acs.est.5b05496 [doi]

PST - ppublish

SO - Environ Sci Technol. 2016 Mar 1;50(5):2381-8. doi: 10.1021/acs.est.5b05496. Epub 2016 Feb 19.

PMID- 26966787

OWN - NLM

STAT- In-Data-Review

DA - 20160406

IS - 1520-5851 (Electronic)

IS - 0013-936X (Linking)

VI - 50

IP - 7

DP - 2016 Apr 5

TI - Nationwide Distribution of Per- and Polyfluoroalkyl Substances in Outdoor Dust in Mainland China From Eastern to Western Areas.

PG - 3676-85

LID - 10.1021/acs.est.6b00649 [doi]

AB - From eastern to western areas, per- and polyfluoroalkyl substances (PFASs) were detected at substantial levels in the outdoor dust across mainland China. Urban samples generally showed higher levels compared with those of rural samples. Compared with neutral PFASs, ionizable PFASs (C4-C12 perfluoroalkyl carboxylic acids and C4/C8 perfluoroalkyl sulfonic acids) were more abundant, with the highest total concentration up to 1.6×10^2 ng/g and perfluorooctanoic acid (PFOA) being a predominant analogue. Fluorotelomer alcohols (FTOHs) and polyfluoroalkyl phosphoric acid diesters (DiPAPs) were both detected in most samples with total concentrations of 0.12-32 and 0.030-20 ng/g, respectively. Perfluorooctane sulfonamidoethanols/sulfonamides (FOSE/As) were detected at low frequencies (<30%). In addition to partitioning to organic moiety, specific adsorption onto mineral particles can be important for PFASs to bind onto outdoor dust, especially for short-chain ionizable PFASs. The eastern plain areas were characterized by a higher contribution of long-chain ionizable PFASs; whereas the western high plateau areas were characterized by the dominating contribution of short-chain analogues. The difference suggests that the long-range atmospheric transport potential of PFASs from source regions to the inland is probably limited by the increase in altitude, and different sources from adjacent regions may influence the western border area of China.

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LA - eng

PT - Journal Article

DEP - 20160323

PL - United States

TA - Environ Sci Technol

JT - Environmental science & technology

JID - 0213155

SB - IM

EDAT- 2016/03/12 06:00

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PHST- 2016/03/23 [aheadofprint]

AID - 10.1021/acs.est.6b00649 [doi]

PST - ppublish

SO - Environ Sci Technol. 2016 Apr 5;50(7):3676-85. doi: 10.1021/acs.est.6b00649. Epub 2016 Mar 23.

PMID- 26900769

OWN - NLM

STAT- In-Data-Review

DA - 20160406

IS - 1520-5851 (Electronic)

IS - 0013-936X (Linking)

VI - 50

IP - 7

DP - 2016 Apr 5

TI - Pesticide Mixture Toxicity in Surface Water Extracts in Snails (*Lymnaea stagnalis*) by an in Vitro Acetylcholinesterase Inhibition Assay and Metabolomics.

PG - 3937-44

LID - 10.1021/acs.est.5b04577 [doi]

AB - Many chemicals in use end up in the aquatic environment. The toxicity of water samples can be tested with bioassays, but a metabolomic approach has the advantage that multiple end points can be measured simultaneously and the affected metabolic pathways can be revealed. A current challenge in metabolomics is the study of mixture effects. This study aims at investigating the toxicity of an environmental extract and its most abundant chemicals identified by target chemical analysis of >100 organic micropollutants and effect-directed analysis (EDA) using the acetylcholinesterase (AChE) bioassay and metabolomics. Surface water from an agricultural area was sampled with a large volume solid phase extraction (LV-SPE) device using three cartridges containing neutral, anionic, and cationic sorbents able to trap several pollutants classes like pharmaceuticals, pesticides, PAHs, PCBs, and perfluorinated surfactants. Targeted chemical analysis and AChE bioassay were performed on the cartridge extracts. The extract

of the neutral sorbent cartridge contained most of the targeted chemicals, mainly imidacloprid, thiacloprid, and pirimicarb, and was the most potent AChE inhibitor. Using an EDA approach, other AChE inhibiting candidates were identified in the neutral extract, such as carbendazim and esprocarb. Additionally, a metabolomics experiment on the central nervous system (CNS) of the freshwater snail *Lymnaea stagnalis* was conducted. The snails were exposed to the extract, the three most abundant chemicals individually, and a mixture of these. The extract disturbed more metabolic pathways than the three most abundant chemicals individually, indicating the contribution of other chemicals. Most pathways perturbed by the extract exposure overlapped with those related to exposure to neonicotinoids, like the polyamine metabolism involved in CNS injuries. Metabolomics for the straightforward comparison between a complex mixture and single compound toxicity is still challenging but, compared to traditional biotesting, is a promising tool due to its increased sensitivity.

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LA - eng

PT - Journal Article

DEP - 20160309

PL - United States

TA - Environ Sci Technol

JT - Environmental science & technology

JID - 0213155

SB - IM

EDAT- 2016/02/24 06:00

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PHST- 2016/03/09 [aheadofprint]
 AID - 10.1021/acs.est.5b04577 [doi]
 PST - ppublish
 SO - Environ Sci Technol. 2016 Apr 5;50(7):3937-44. doi: 10.1021/acs.est.5b04577. Epub 2016 Mar 9.

PMID- 26894610
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160406
 IS - 1520-5851 (Electronic)
 IS - 0013-936X (Linking)
 VI - 50
 IP - 7
 DP - 2016 Apr 5
 TI - Effects of Aqueous Film-Forming Foams (AFFFs) on Trichloroethene (TCE) Dechlorination by a Dehalococcoides mccartyi-Containing Microbial Community.
 PG - 3352-61
 LID - 10.1021/acs.est.5b04773 [doi]
 AB - The application of aqueous film-forming foams (AFFFs) to extinguish chlorinated solvent-fueled fires has led to the co-contamination of poly- and perfluoroalkyl substances (PFASs) and trichloroethene (TCE) in groundwater and soil. Although reductive dechlorination of TCE by Dehalococcoides mccartyi is a frequently used remediation strategy, the effects of AFFF and PFASs on TCE dechlorination are not well-understood. Various AFFF formulations, PFASs, and ethylene glycols were amended to the growth medium of a D. mccartyi-containing enrichment culture to determine the impact on dechlorination, fermentation, and methanogenesis. The community was capable of fermenting organics (e.g., diethylene glycol butyl ether) in all AFFF formulations to hydrogen and acetate, but the product concentrations varied significantly according to formulation. TCE was dechlorinated in the presence of an AFFF formulation manufactured by 3M but was not dechlorinated in the presence of formulations from two other manufacturers. Experiments amended with AFFF-derived PFASs and perfluoroalkyl acids (PFAAs) indicated that dechlorination could be inhibited by PFASs but that the inhibition depends on surfactant concentration and structure. This study revealed that the fermentable components of AFFF can stimulate TCE dechlorination, while some of the fluorinated compounds in certain AFFF formulations can inhibit dechlorination.

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LA - eng

PT - Journal Article

DEP - 20160321

PL - United States

TA - Environ Sci Technol

JT - Environmental science & technology

JID - 0213155

SB - IM

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AID - 10.1021/acs.est.5b04773 [doi]

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SO - Environ Sci Technol. 2016 Apr 5;50(7):3352-61. doi: 10.1021/acs.est.5b04773. Epub
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PMID- 25258305

OWN - NLM

STAT- In-Data-Review

DA - 20160211

IS - 1522-7278 (Electronic)

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VI - 31

IP - 3

DP - 2016 Mar

TI - Developmental toxicity and DNA damage to zebrafish induced by perfluorooctane
sulfonate in the presence of ZnO nanoparticles.

PG - 360-71

LID - 10.1002/tox.22050 [doi]

AB - Perfluorooctane sulfonate (PFOS) and ZnO nanoparticles (ZnO-NPs) are frequently
detected in the environment, but few studies have assessed their joint toxicity.

In this study, the acute toxicity and chronic toxicity to zebrafish (*Danio rerio*) induced by PFOS in the presence of ZnO-NPs were investigated, including developmental toxicity and DNA damage. The embryos were exposed to PFOS (only) (0.4, 0.8, and 1.6 mg/L) and PFOS plus ZnO-NPs (0.4 + 50, 0.8 + 50, and 1.6 + 50 mg/L) solutions to evaluate mortality (96 h), body length (96 h), hatch rate (72 h), heart rate (48 h), and malformation rate (96 h). The results revealed that the co-treatment could cause more severe developmental toxicity compared with the control and single-treatments, and the toxic effects generally increased in a dose-response manner. In addition, adult zebrafish were exposed to single and mixed solutions of PFOS and ZnO-NPs (at the concentrations mentioned above) for 30 days. DNA damage to zebrafish was evaluated by the comet assay and micronucleus test. We found that the PFOS single-treatment at all doses (0.4, 0.8, and 1.6 mg/L) could strongly induce DNA damage to peripheral blood cells and that ZnO-NPs could aggravate the formation of DNA damage in co-treatments. Histological examination of liver, testicle, and ovary showed that the presence of ZnO-NPs (50 mg/L) could also cause more serious histological damage to adult zebrafish than PFOS alone. As a result, the synergistic effects played an important role during joint exposure. Our observations provide a basic understanding of the joint toxicity of PFOS and ZnO-NPs to aquatic organisms. (c) 2014 Wiley Periodicals, Inc. *Environ Toxicol* 31: 360-371, 2016.

CI - (c) 2014 Wiley Periodicals, Inc.

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LA - eng

PT - Journal Article

DEP - 20140925
 PL - United States
 TA - Environ Toxicol
 JT - Environmental toxicology
 JID - 100885357
 SB - IM
 OTO - NOTNLM
 OT - DNA damage
 OT - ZnO nanoparticles
 OT - comet assay
 OT - micronucleus
 OT - perfluorooctane sulfonate
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 SO - Environ Toxicol. 2016 Mar;31(3):360-71. doi: 10.1002/tox.22050. Epub 2014 Sep 25.

PMID- 26383989
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160419
 IS - 1552-8618 (Electronic)
 IS - 0730-7268 (Linking)
 VI - 35
 IP - 5
 DP - 2016 May
 TI - Competing mechanisms for perfluoroalkyl acid accumulation in plants revealed using an Arabidopsis model system.
 PG - 1138-47
 LID - 10.1002/etc.3251 [doi]
 AB - Perfluoroalkyl acids (PFAAs) bioaccumulate in plants, presenting a human exposure route if present in irrigation water. Curiously, accumulation of PFAAs in plant tissues is greatest for both the short-chain and long-chain PFAAs, generating a U-shaped relationship with chain length. In the present study, the authors decouple competing mechanisms of PFAA accumulation using a hydroponic model plant system (*Arabidopsis thaliana*) exposed to a suite of 10 PFAAs to determine uptake, depuration, and translocation kinetics. Rapid saturation of root concentrations occurred for all PFAAs except perfluorobutanoate, the least-sorptive (shortest-chain) PFAA. Shoot concentrations increased continuously, indicating that PFAAs are efficiently transported and accumulate in shoots. Tissue concentrations of PFAAs during depuration rapidly declined in roots but remained constant in shoots, demonstrating irreversibility of the translocation process.

Root and shoot concentration factors followed the U-shaped trend with perfluoroalkyl chain length; however, when normalized to dead-tissue sorption, this relationship linearized. The authors therefore introduce a novel term, the "sorption normalized concentration factor," to describe PFAA accumulation in plants; because of their hydrophobicity, sorption is the determining factor for long-chain PFAAs, whereas the shortest-chain PFAAs are most effectively transported in the plant. The present study provides a mechanistic explanation for previously unexplained PFAA accumulation trends in plants and suggests that shorter-chained PFAAs may bioaccumulate more readily in edible portions. Environ Toxicol Chem 2016;35:1138-1147. (c) 2015 SETAC.

CI - (c) 2015 SETAC.

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LA - eng

PT - Journal Article

DEP - 20160304

PL - United States
TA - Environ Toxicol Chem
JT - Environmental toxicology and chemistry / SETAC
JID - 8308958
SB - IM
OTO - NOTNLM
OT - Bioaccumulation
OT - Environmental fate
OT - Perfluoroalkyl substance
OT - Plant
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SO - Environ Toxicol Chem. 2016 May;35(5):1138-47. doi: 10.1002/etc.3251. Epub 2016 Mar 4.

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OWN - NLM
STAT- In-Data-Review
DA - 20160229
IS - 1552-8618 (Electronic)
IS - 0730-7268 (Linking)
VI - 35
IP - 3
DP - 2016 Mar
TI - Toxicokinetics of perfluorooctane sulfonate in rainbow trout (*Oncorhynchus mykiss*).
PG - 717-27
LID - 10.1002/etc.3230 [doi]
AB - Rainbow trout (*Oncorhynchus mykiss*) confined to respirometer-metabolism chambers were dosed with perfluorooctane sulfonate (PFOS) by intra-arterial injection and sampled to obtain concentration time-course data for plasma and either urine or expired water. The data were then analyzed using a 2-compartment clearance-volume model. Renal and branchial clearance rates (mL/d/kg) determined for all experiments averaged 19% and 81% of total clearance, respectively. Expressed as mean values for all experiments, the steady-state volume of distribution was 277 mL/kg and the terminal half-life was 86.8 d. Additional animals were exposed to PFOS in water, resulting in an average calculated branchial uptake efficiency of 0.36%. The renal clearance rate determined in the present study is approximately 75 times lower than that determined in earlier studies with perfluorooctanoate (PFOA). Previously, it was suggested that PFOA is a substrate for membrane transporters in the trout kidney. The present study suggests that glomerular

filtration may be sufficient to explain the observed renal clearance rate for PFOS, although a role for membrane transporters cannot be ruled out. These findings demonstrate that models developed to predict the bioaccumulation of perfluoroalkyl acids by fish must account for differences in renal clearance of individual compounds. Environ Toxicol Chem 2016;35:717-727. (c) 2015 SETAC.

CI - (c) 2015 SETAC.

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LA - eng

PT - Journal Article

DEP - 20160209

PL - United States

TA - Environ Toxicol Chem

JT - Environmental toxicology and chemistry / SETAC

JID - 8308958

SB - IM

OTO - NOTNLM

OT - Bioaccumulation

OT - Perfluorooctane sulfonate

OT - Renal elimination

OT - Tissue distribution

OT - Toxicokinetics

EDAT- 2015/09/04 06:00

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PHST- 2015/08/01 [revised]
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AID - 10.1002/etc.3230 [doi]
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SO - Environ Toxicol Chem. 2016 Mar;35(3):717-27. doi: 10.1002/etc.3230. Epub 2016 Feb 9.

PMID- 26918744

OWN - NLM

STAT- In-Data-Review

DA - 20160227

IS - 1468-1331 (Electronic)

IS - 1351-5101 (Linking)

VI - 23

IP - 3

DP - 2016 Mar

TI - The diagnostic yield of transesophageal echocardiography in patients with cryptogenic cerebral ischaemia: a meta-analysis.

PG - 569-79

LID - 10.1111/ene.12897 [doi]

AB - BACKGROUND AND PURPOSE: The diagnostic utility of transesophageal echocardiography (TEE) in patients with cryptogenic ischaemic stroke (IS) or transient ischaemic attack (TIA) remains controversial. METHODS: A systematic review and meta-analysis was performed according to PRISMA guidelines to estimate the pooled prevalence of potential cardioembolic causes detected by TEE in prospective observational studies of cryptogenic IS/TIA. Cardiac conditions causally associated with cerebral ischaemia were considered to be intramural thrombi and intracardiac tumors according to ASCO phenotyping of IS. RESULTS: Thirty-five eligible studies, comprising 5772 patients (mean age 53.6 years, 56.9% men) were identified. The most common TEE finding was ascending aorta and/or aortic arch atheroma [51.2% (27.4%-74.5%)], followed by patent foramen ovale (PFO) [43.2% (36.3%-50.4%)]. Complex aortic plaques and large PFOs were reported in 14% (10.2%-18.9%) and 19.5% (16.6%-22.8%) of TEE evaluations. The prevalence of atrial septal aneurysm was 12.3% (7.9%-18.7%) and was significantly higher in conjunction with PFO presence (risk ratio 2.04, 95% confidence interval 1.63-2.54, $P < 0.001$). The prevalence of left atrial thrombus [3.0% (1.1%-8.3%)] and spontaneous echo contrast [3.8% (2.3%-6.2%)] was low. The prevalence of intracardiac tumors was extremely uncommon [0.2% (0%-0.7%)]. Significant heterogeneity was identified ($I(2) > 60\%$) in the majority of analyses. Heterogeneity was not affected by cryptogenic stroke definition (TOAST versus alternative criteria). After dichotomizing available studies using a cut-off of 50 years, PFO was significantly ($P = 0.001$) more prevalent in younger than in older patients. CONCLUSION: Routine TEE in patients with cryptogenic IS/TIA commonly identifies abnormal findings. However, the prevalence of cardiac conditions considered to be causally associated with cerebral ischaemia

(intracardiac thrombi and tumors) is low.

CI - (c) 2015 EAN.

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 LA - eng
 PT - Journal Article
 DEP - 20151119
 PL - England
 TA - Eur J Neurol
 JT - European journal of neurology
 JID - 9506311
 SB - IM
 OTO - NOTNLM
 OT - cryptogenic
 OT - stroke
 OT - transesophageal echocardiography
 OT - transient ischaemic attack
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 PMID- 26980645
 OWN - NLM
 STAT- Publisher
 DA - 20160316
 LR - 20160318
 IS - 1879-0267 (Electronic)
 IS - 0020-1383 (Linking)
 DP - 2016 Mar 4
 TI - Surgical tips of intramedullary nailing in severely bowed femurs in atypical femur fractures: Simulation with 3D printed model.
 LID - S0020-1383(16)30025-0 [pii]
 LID - 10.1016/j.injury.2016.02.026 [doi]
 AB - INTRODUCTION: The surgical management of atypical femoral fractures (AFFs) is

complex in cases with severe bowing of the femur, being associated with a high rate of failure. Our first aim was to use preoperative templating and 3D printed model characterise the technical difficulties associated with use of current commercially available intramedullary nail (IMN) systems for the management of AFFs with severe bowing. Our second aim was to use outcomes of our 3D printing analysis to define technical criteria to overcome these problems. MATERIAL AND METHODS: The modelled femur with 3D printing had an anterior bowing curvature radius of 772mm and an angle of lateral bowing of 15.4 degrees . Nine commercially available IMN systems were evaluated in terms of position of the nail within the medullary canal, occurrence of perforation of femoral cortex by the distal tip of the nail, and location of the site of perforation relative to the knee joint. The following IMN systems were evaluated: unreamed femoral nail (UFN), cannulated femoral nail (CFN), Sirius nail, right and left expert Asian femoral nail (A2FN), right and left Zimmer Natural Nail (ZNN), proximal femoral nail anti-rotation (PFNA), and Zimmer Cephalomedullary Nail (CMN). RESULTS: Along the sagittal plane, the UFN, CFN and Sirius systems were acceptably contained within the medullary canal, as well as the "opposite side" A2FN and ZNN. Only the Sirius IMN system was contained along the coronal plane. The distal part of the all other IMN systems perforated the anterior cortex of the femur, at distances ranging between 2.8 and 11.7cm above the distal end of the femoral condyles. Using simulated fracture reduction in the 3D printed model, none of the 9 IMN systems provided acceptable anatomical reduction of the fracture. A residual gap in fragment position and translation was provided by the "opposite side" ZNN, followed by the UFN and Sirius systems. CONCLUSION: Commercially available IMN systems showed mismatch with severely bowed femurs. Our simulation supports that fit of these systems can be improved using an IMN system with a small radius of curvature and diameter, and by applying specific operative procedures.

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LA - ENG
 PT - JOURNAL ARTICLE
 DEP - 20160304
 TA - Injury
 JT - Injury
 JID - 0226040
 OTO - NOTNLM
 OT - 3D print
 OT - Atypical femur fracture
 OT - Femur
 OT - Intramedullary nailing
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 PMID- 26803696
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 DA - 20160313
 IS - 1879-0267 (Electronic)
 IS - 0020-1383 (Linking)
 VI - 47
 IP - 3
 DP - 2016 Mar
 TI - Lacking evidence for performance of implants used for proximal femoral fractures
 - A systematic review.
 PG - 586-94
 LID - 10.1016/j.injury.2016.01.001 [doi]
 LID - S0020-1383(16)00003-6 [pii]
 AB - INTRODUCTION: Evaluation of the long-term performance of implants used in trauma surgery relies on post-marked clinical studies since no registry based implant assessment exists. The purpose of this study was to evaluate the evidence of performance of implants currently used for treating proximal femoral fractures (PFF) in Denmark. METHOD: PubMed was searched for clinical studies on primary PFF with follow-up >=12 months, reporting implant-related failure and evaluating one of following: DHS, CHS, HipLoc, Gamma3, IMHS, InterTan, PFN, PFNA or PTN. LIMITS: English language and publication date after 1st of January 1990. RESULTS: All studies were evidence level II or III. 30 publications for SHS were found: 13 of CHS, 15 of DHS and 2 of HipLoc. In total CHS was evaluated in 1110 patients (900 prospectively), DHS in 2486 (567 prospectively) and HipLoc in 251 (all

prospectively). Fifty-four publications for nails were found: 13 of Gamma3, 7 of IMHS, 5 of InterTan, 10 of PFN, 24 of PFNA and 0 of PTN. In total Gamma3 was evaluated in 1088 patients (829 prospectively), IMHS in 1543 (210 prospectively), InterTan in 595 (585 prospectively), PFN in 716 (557 prospectively), PFNA in 1762 (1018 prospectively) and PTN in 0. CONCLUSIONS: The clinical evidence behind the current implants used for proximal femoral fractures is weak considering the number of implants used worldwide. Sporadic evaluation is not sufficient to identify long term problems. A systematic post market surveillance of implants used for fracture treatment, preferable by a national register, is necessary in the future.

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LA - eng

PT - Journal Article

PT - Review

DEP - 20160113

PL - Netherlands

TA - Injury

JT - Injury

JID - 0226040

SB - IM

OTO - NOTNLM

OT - Hip fracture

OT - Implant failure

OT - Implant survival

OT - Proximal femoral fracture

OT - Reoperation

OT - Trochanteric fracture

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 PMID- 26614251
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 DA - 20160201
 IS - 1618-131X (Electronic)
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 VI - 219
 IP - 2
 DP - 2016 Mar
 TI - Levels of persistent contaminants in relation to fish consumption among older male anglers in Wisconsin.
 PG - 184-94
 LID - 10.1016/j.ijheh.2015.11.001 [doi]
 LID - S1438-4639(15)00139-X [pii]
 AB - Fish are an important source of nutrients which may reduce risk of adverse health outcomes such as cardiovascular disease; however, fish may also contain significant amounts of environmental pollutants such as mercury, polychlorinated biphenyls (PCBs), polybrominated diphenyl ethers (PBDEs), and perfluorinated compounds (PFCs, also called perfluoroalkyl compounds), which confer increased risk for adverse health effects. The Wisconsin Departments of Health Services and Natural Resources developed a survey instrument, along with a strategy to collect human biological samples to assess the risks and benefits associated with long-term fish consumption among older male anglers in Wisconsin. The target population was men aged 50 years and older, who fish Wisconsin waters and live in the state of Wisconsin. Participants provided blood and hair samples and completed a detailed (paper) questionnaire, which included questions on basic demographics, health status, location of catch and species of fish caught/eaten, consumption of locally caught and commercially purchased fish, and awareness and source of information for local and statewide consumption guidelines. Biological samples were used to assess levels of PCBs, PBDEs, PFCs (blood), and mercury (hair and blood). Quantile regression analysis was used to investigate the associations between biomarker levels and self-reported consumption of fish from the Great Lakes and other areas of concern, other locally caught fish, and commercially purchased fish (meals per year). Respondents had a median age of 60.5 (interquartile range: 56, 67) years. The median fish consumption was 54.5

meals per year, with most fish meals coming from locally-caught fish. Participants had somewhat higher mercury levels compared with the US general population, while levels of other contaminants were similar or lower. Multivariate regression models showed that consumption of fish from the Great Lakes and areas of concern was associated with higher levels of each of the contaminants with the exception of PBDEs, as was consumption of locally caught fish from other water bodies. All commercial fish consumption was also associated with both hair and blood mercury. When looking at specific PCB, PBDE and PFC analytes, consumption of fish from the Great Lakes and areas of concern was associated with higher levels of each of the individual PCB congeners examined, as well as higher levels of all of the PFCs examined, with the exception of PFHxS. Among the PFCs, locally caught fish from other water bodies was also associated with higher levels of each of the congeners examined except PFHxS. Finally, all commercial fish was associated with higher levels of PFHxS.

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LA - eng

PT - Journal Article

DEP - 20151110

PL - Germany

TA - Int J Hyg Environ Health

JT - International journal of hygiene and environmental health

JID - 100898843

SB - IM

OTO - NOTNLM

OT - Anglers
 OT - Fish consumption
 OT - Great lakes
 OT - Persistent
 OT - Pollutant
 EDAT- 2015/11/29 06:00
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 SO - Int J Hyg Environ Health. 2016 Mar;219(2):184-94. doi:
 10.1016/j.ijheh.2015.11.001. Epub 2015 Nov 10.

 PMID- 26931527
 OWN - NLM
 STAT- Publisher
 DA - 20160317
 LR - 20160317
 IS - 1520-5126 (Electronic)
 IS - 0002-7863 (Linking)
 DP - 2016 Mar 17
 TI - Fluorine-Terminated Diamond Surfaces as Dense Dipole Lattices: The Electrostatic Origin of Polar Hydrophobicity.
 AB - Despite the pronounced polarity of C-F bonds, many fluorinated carbon compounds are hydrophobic: a controversial phenomenon known as "polar hydrophobicity". Here, its underlying microscopic mechanisms are explored by ab initio calculations of fluorinated and hydrogenated diamond (111) surfaces interacting with single water molecules. Gradient- and van der Waals-corrected density functional theory simulations reveal that "polar hydrophobicity" of the fully fluorinated surfaces is caused by a negligible surface/water electrostatic interaction. The densely packed C-F surface dipoles generate a short-range electric field that decays within the core repulsion zone of the surface and hence vanishes in regions accessible by adsorbates. As a result, water physisorption on fully F-terminated surfaces is weak (adsorption energies $E_{ad} < 0.1$ eV) and dominated by van der Waals interactions. Conversely, the near-surface electric field generated by loosely packed dipoles on mixed F/H-terminated surfaces has a considerably longer range, resulting in a stronger water physisorption ($E_{ad} > 0.2$ eV) that is dominated by electrostatic interactions. The suppression of electrostatic interactions also holds for perfluorinated molecular carbon compounds, thus explaining the prevalent hydrophobicity of fluorocarbons. In general, densely packed polar terminations do not always lead to short-range electric fields. For example, surfaces with substantial electron density spill-out give rise to electric fields with a much slower decay. However,

electronic spill-out is limited in F/H-terminated carbon materials. Therefore, our ab initio results can be reproduced and rationalized by a simple classical point-charge model. Consequently, classical force fields can be used to study the wetting of F/H-terminated diamond, revealing a pronounced correlation between adsorption energies of single H₂O molecules and water contact angles.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20160317

TA - J Am Chem Soc

JT - Journal of the American Chemical Society

JID - 7503056

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AID - 10.1021/jacs.5b04073 [doi]

PST - aheadofprint

SO - J Am Chem Soc. 2016 Mar 17.

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OWN - NLM

STAT- Publisher

DA - 20160328

LR - 20160329

IS - 1099-1263 (Electronic)

IS - 0260-437X (Linking)

DP - 2016 Mar 28

TI - Perfluorooctane sulfonate (PFOS) impairs the proliferation of C17.2 neural stem cells via the downregulation of GSK-3beta/beta-catenin signaling.

LID - 10.1002/jat.3320 [doi]

AB - The neurotoxic effects of perfluorooctane sulfonate (PFOS) have attracted significant research attention in recent years. In the present study, we investigated the impact of PFOS exposure on the physiology of neural stem cells (NSCs) in vitro. We showed that PFOS exposure markedly attenuated the proliferation of C17.2 neural stem cells in both dose- and time-dependent manners. Additionally, we found that PFOS decreased Ser9 phosphorylation of glycogen synthase kinase-3beta (pSer9-GSK-3beta), leading to the activation of GSK-3beta and resultant downregulation of cellular beta-catenin. Furthermore, blockage of GSK-3beta with lithium chloride significantly attenuated both the PFOS-induced downregulation of GSK-3beta/beta-catenin and the proliferative impairment of C17.2 cells. Notably, the expression of various downstream targets was altered accordingly, such as c-myc, cyclin D1 and survivin. In conclusion, the present study demonstrated that PFOS decreased the proliferation of C17.2 cells via the negative modulation of the GSK-3beta/beta-catenin pathway. We present the potential mechanisms underlying the PFOS-induced toxic effects on NSCs to provide novel insights into the neurotoxic mechanism of PFOS. Copyright (c) 2016 John Wiley & Sons, Ltd.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20160328

TA - J Appl Toxicol
JT - Journal of applied toxicology : JAT
JID - 8109495
OTO - NOTNLM
OT - Wnt/beta-catenin signaling
OT - neural stem cells (NSCs)
OT - neurotoxicology
OT - perfluorooctane sulfonate (PFOS)
OT - proliferation
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OWN - NLM

STAT- In-Data-Review

DA - 20160419

IS - 1873-3778 (Electronic)

IS - 0021-9673 (Linking)

VI - 1445

DP - 2016 May 6

TI - A fast and sensitive method for the simultaneous analysis of a wide range of per- and polyfluoroalkyl substances in indoor dust using on-line solid phase extraction-ultrahigh performance liquid chromatography-time-of-flight-mass spectrometry.

PG - 36-45

LID - 10.1016/j.chroma.2016.03.058 [doi]

LID - S0021-9673(16)30340-5 [pii]

AB - A fast and sensitive method for simultaneous determination of 18 traditional and 6 alternative per- and polyfluoroalkyl substances (PFASs) using solid-liquid extraction (SLE), off-line clean-up using activated carbon and on-line solid phase extraction-ultrahigh performance liquid chromatography-time-of-flight-mass spectrometry (on-line SPE-UHPLC-TOF-MS) was developed. The extraction efficiency was studied and recoveries in range the 58-114% were obtained. Extraction and injection volumes were also optimized to 2mL and 400muL, respectively. The method was validated by spiking dust from a vacuum cleaner bag that had been found to contain low levels of the PFASs in focus. Low method detection limits (MDLs) and method quantification limits (MQLs) in the range 0.008-0.846ngg(-1) and 0.027-2.820ngg(-1) were obtained, respectively. For most of the PFASs, the accuracies were between 70 and 125% in the range from 2 to100ngg(-1) dust. Intra-day and inter-day precisions were in general well below 30%. Analysis of a Standard Reference Material (SRM 2585) showed high accordance with results

obtained by other laboratories. Finally, the method was applied to seven indoor dust samples, and PFAS concentrations in the range 0.02-132ngg(-1) were found. The highest median concentrations were observed for some of the alternative PFASs, such as 6:2-diPAP (25ngg(-1)), 8:2-diPAP (49ngg(-1)), and PFOPA (23ngg(-1)), illustrating the importance of inclusion of new PFASs in the analytical methods.

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LA - eng

PT - Journal Article

DEP - 20160324

PL - Netherlands

TA - J Chromatogr A

JT - Journal of chromatography. A

JID - 9318488

SB - IM

OTO - NOTNLM

OT - Analysis

OT - Indoor dust

OT - PAPs

OT - PFASs

OT - PFOA

OT - PFOS

OT - PFPAs

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PST - ppublish

SO - J Chromatogr A. 2016 May 6;1445:36-45. doi: 10.1016/j.chroma.2016.03.058. Epub 2016 Mar 24.

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OWN - NLM

STAT- In-Data-Review

DA - 20160301

IS - 1873-3778 (Electronic)

IS - 0021-9673 (Linking)

VI - 1438

DP - 2016 Mar 18

TI - Multiresidue analysis of endocrine-disrupting compounds and perfluorinated sulfates and carboxylic acids in sediments by ultra-high-performance liquid chromatography-tandem mass spectrometry.

PG - 133-42

LID - 10.1016/j.chroma.2016.02.022 [doi]

LID - S0021-9673(16)30108-X [pii]

AB - A multiresidue analytical method for the determination of 11 perfluorinated compounds and 22 endocrine-disrupting compounds (ECDs) including 13 natural and synthetic estrogens (free and conjugated forms), 2 alkylphenols, 1 plasticiser, 2 UV-filters, 1 antimicrobial, and 2 organophosphorus compounds in sediments has been developed. Ultrasound-assisted extraction followed by solid phase extraction (SPE) with graphitized carbon black (GCB) cartridge as clean-up step were used. The extraction process yield was optimized in terms of solvent composition. Then, a 3(2) experimental design was used to optimize solvent volume and sonication time by response surface methodology, which simplifies the optimization procedure. The final extract was analyzed by ultra-high performance liquid chromatography coupled with tandem mass spectrometry. The optimized sample preparation method is simple and robust, and allows recovery of ECDs belonging to different classes in a complex matrix such as sediment. The use of GCB for SPE allowed to obtain with a single clean-up procedure excellent recoveries ranging between 75 and 110% (relative standard deviation <16%). The developed methodology has been successfully applied to the analysis of ECDs in sediments from different rivers and lakes of the Lazio Region (Italy). These analyses have shown the ubiquitous presence of chloro-substituted organophosphorus flame retardants and bisphenol A, while other analyzed compounds were occasionally found at concentration between the limit of detection and quantification.

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 LA - eng
 PT - Journal Article
 DEP - 20160208
 PL - Netherlands
 TA - J Chromatogr A
 JT - Journal of chromatography. A
 JID - 9318488
 SB - IM
 OTO - NOTNLM
 OT - Endocrine-disrupting compounds
 OT - Experimental design
 OT - Graphitized carbon black
 OT - Liquid chromatography-mass spectrometry (LC-MS)
 OT - Sediments
 OT - Solid phase extraction (SPE)
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 AID - 10.1016/j.chroma.2016.02.022 [doi]
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 SO - J Chromatogr A. 2016 Mar 18;1438:133-42. doi: 10.1016/j.chroma.2016.02.022. Epub 2016 Feb 8.

 PMID- 26949215
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160322
 IS - 1873-3778 (Electronic)
 IS - 0021-9673 (Linking)
 VI - 1441
 DP - 2016 Apr 8
 TI - A water resistant solid-phase microextraction fiber with high selectivity prepared by a metal organic framework with perfluorinated pores.
 PG - 16-23
 LID - 10.1016/j.chroma.2016.02.076 [doi]
 LID - S0021-9673(16)30221-7 [pii]

AB - A novel solid-phase microextraction (SPME) fiber was fabricated by the construction of fluororous metal organic frameworks (FMOF) and a polyimide (PI) composite strategy. As an auxiliary material, PI was expected to help FMOF particles form well-knit film on the surface of stainless steel wire and reinforce the coating, and FMOF was expected to afford a special structure to absorb, extract and enrich. Furthermore, it was explored for the headspace SPME (HS-SPME) of six volatile aromatic compounds (VACs) from water samples followed by gas chromatographic (GC) separation with flame ionization detection. Under the optimized conditions, the fiber afforded wide linear ranges ($1-1000\mu\text{g L}^{-1}$), low detection limits ($0.15-0.9\mu\text{g L}^{-1}$) and acceptable repeatability ($<4.6\%$) and reproducibility ($<7.3\%$). The FMOF@PI coated fiber not only offered large enhancement factors for benzene (1227) but also exhibited high extraction selectivity for benzene to other benzene homologues, hydrocarbons and phenols; for example, the extraction ratio of benzene to toluene, n-hexane and phenol could be as high as 10.2, 64.1 and 32.3, respectively. Moreover, the FMOF@PI-coated fiber afforded good thermal, water and organic solvent stabilities, and a long lifetime (over 200 times). The developed method was successfully applied to the determination of VACs in wastewater samples.

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 LA - eng
 PT - Journal Article
 DEP - 20160303
 PL - Netherlands
 TA - J Chromatogr A
 JT - Journal of chromatography. A
 JID - 9318488
 SB - IM
 OTO - NOTNLM
 OT - Fluorine-lined
 OT - Hydrophobic
 OT - Metal organic framework
 OT - Selective extraction
 OT - Solid-phase microextraction
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 2016 Mar 3.

 PMID- 27016113
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160406
 IS - 1873-3778 (Electronic)
 IS - 0021-9673 (Linking)
 VI - 1443
 DP - 2016 Apr 22
 TI - Immobilized metal affinity chromatography on collapsed Langmuir-Blodgett
 iron(III) stearate films and iron(III) oxide nanoparticles for bottom-up
 phosphoproteomics.
 PG - 181-90
 LID - 10.1016/j.chroma.2016.03.044 [doi]
 LID - S0021-9673(16)30309-0 [pii]
 AB - Phosphorylation is the enzymatic reaction of site-specific phosphate transfer
 from energy-rich donors to the side chains of serine, threonine, tyrosine, and
 histidine residues in proteins. In living cells, reversible phosphorylation
 underlies a universal mechanism of intracellular signal transduction. In this

context, analysis of the phosphoproteome is a prerequisite to better understand the cellular regulatory networks. Conventionally, due to the low contents of signaling proteins, selective enrichment of proteolytic phosphopeptides by immobilized metal affinity chromatography (IMAC) is performed prior to their LC-MS or -MS/MS analysis. Unfortunately, this technique still suffers from low selectivity and compromised analyte recoveries. To overcome these limitations, we propose IMAC systems comprising stationary phases based on collapsed Langmuir-Blodgett films of iron(III) stearate (FF) or iron(III) oxide nanoparticles (FO) and mobile phases relying on ammonia, piperidine and heptadecafluorooctanesulfonic acid (PFOS). Experiments with model phosphopeptides and phosphoprotein tryptic digests showed superior binding capacity, selectivity and recovery for both systems in comparison to the existing commercial analogs. As evidenced by LC-MS/MS analysis of the HeLa phosphoproteome, these features of the phases resulted in increased phosphoproteome coverage in comparison to the analogous commercially available phases, indicating that our IMAC protocol is a promising chromatographic tool for in-depth phosphoproteomic research.

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 LA - eng
 PT - Journal Article
 DEP - 20160319
 PL - Netherlands
 TA - J Chromatogr A
 JT - Journal of chromatography. A
 JID - 9318488
 SB - IM
 OTO - NOTNLM
 OT - Immobilized metal affinity chromatography (IMAC)
 OT - Iron oxide
 OT - Langmuir-Blodgett films
 OT - Perfluorooctanoic acid
 OT - Phosphopeptides
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 AID - 10.1016/j.chroma.2016.03.044 [doi]
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 SO - J Chromatogr A. 2016 Apr 22;1443:181-90. doi: 10.1016/j.chroma.2016.03.044. Epub
 2016 Mar 19.
 PMID- 27038281
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160411
 IS - 1095-7103 (Electronic)
 IS - 0021-9797 (Linking)
 VI - 472
 DP - 2016 Jun 15
 TI - Incorporation of negatively charged iron oxide nanoparticles in the shell of

anionic surfactant-stabilized microbubbles: The effect of NaCl concentration.

PG - 180-6

LID - 10.1016/j.jcis.2016.02.016 [doi]

LID - S0021-9797(16)30096-0 [pii]

AB - We report on the key effect of NaCl for the stabilization of nanoparticle-decorated microbubbles coated by an anionic perfluoroalkylated phosphate $\text{C}_{10}\text{F}_{21}(\text{CH}_2)_2\text{OP}(\text{O})(\text{OH})_2$ surfactant and negatively charged iron oxide nanoparticles. We show that hollow microspheres with shells of 100-200nm in thickness can be stabilized even at high pH when a strong ionic force is required to screen the negative charges. Due to the more drastic conditions required to stabilize the hollow microspheres, they appear to be stable enough to be deposited on a surface and dried. That can be a simple way to fabricate porous ceramics.

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LA - eng

PT - Journal Article

DEP - 20160330

PL - United States

TA - J Colloid Interface Sci

JT - Journal of colloid and interface science

JID - 0043125
SB - IM
OTO - NOTNLM
OT - Bi-modal contrast agent
OT - Hollow microspheres
OT - Magnetic microbubbles
OT - Magnetic nanoparticles
OT - Perfluoroalkyl surfactant
OT - Salt effect
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AID - S0021-9797(16)30096-0 [pii]
AID - 10.1016/j.jcis.2016.02.016 [doi]
PST - ppublish
SO - J Colloid Interface Sci. 2016 Jun 15;472:180-6. doi: 10.1016/j.jcis.2016.02.016.
Epub 2016 Mar 30.

PMID- 26931238
OWN - NLM
STAT- Publisher
DA - 20160302
LR - 20160305
IS - 1096-987X (Electronic)
IS - 0192-8651 (Linking)
DP - 2016 Mar 1
TI - Complexes of adamantane-based group 13 Lewis acids and superacids: Bonding analysis and thermodynamics of hydrogen splitting.
LID - 10.1002/jcc.24328 [doi]
AB - The electronic structure and chemical bonding in donor-acceptor complexes formed by group 13 element adamantane and perfluorinated adamantane derivatives EC9 R'15 (E = B, Al; R' = H, F) with Lewis bases XR3 and XC9 H15 (X = N, P; R= H, CH3) have been studied using energy decomposition analysis at the BP86/TZ2P level of theory. Larger stability of complexes with perfluorinated adamantane derivatives is mainly due to better electrostatic and orbital interactions. Deformation energies of the fragments and Pauli repulsion are of less importance, with exception for the boron-phosphorus complexes. The MO analysis reveals that LUMO energies of EC9 R'15 significantly decrease upon fluorination (by 4.7 and 3.6 eV for E = B and Al, respectively) which results in an increase of orbital interaction energies by 27-38 (B) and 15-26 (Al) kcal mol⁻¹ . HOMO energies of XR3 increase in order PH3 < NH3 < PMe3 < PC9 H15 < NMe3 < NC9 H15 . For the studied complexes, there is a linear correlation between the dissociation energy of the complex and the energy difference between HOMO of the donor and LUMO of the acceptor. The fluorination of the Lewis acid significantly reduces standard

enthalpies of the heterolytic hydrogen splitting $H_2 + D + A = [HD]^+ + [HA]^-$. Analysis of several types of the $[HD]^+ \dots [HA]^-$ ion pair formation in the gas phase reveals that structures with additional H...F interactions are energetically favorable. Taking into account the ion pair formation, hydrogen splitting is predicted to be highly exothermic in case of the perfluorinated derivatives both in the gas phase and in solution. Thus, fluorinated adamantane-based Lewis superacids are attractive synthetic targets for the construction of the donor-acceptor cryptands. (c) 2016 Wiley Periodicals, Inc.

CI - (c) 2016 Wiley Periodicals, Inc.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20160301

TA - J Comput Chem

JT - Journal of computational chemistry

JID - 9878362

OTO - NOTNLM

OT - EDA

OT - aluminum

OT - bonding analysis

OT - boron

OT - donor-acceptor complexes

OT - hydrogen splitting

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AID - 10.1002/jcc.24328 [doi]
PST - aheadofprint
SO - J Comput Chem. 2016 Mar 1. doi: 10.1002/jcc.24328.

PMID- 26980678
OWN - NLM
STAT- In-Data-Review
DA - 20160412
IS - 1532-4117 (Electronic)
VI - 51
IP - 7
DP - 2016 Jun 6
TI - Aqueous phase hydration and hydrate acidity of perfluoroalkyl and n:2
fluorotelomer aldehydes.
PG - 579-82
LID - 10.1080/10934529.2016.1141625 [doi]
AB - The SPARC software program and comparative density functional theory (DFT)
calculations were used to investigate the aqueous phase hydration equilibrium
constants (K_{hyd}) of perfluoroalkyl aldehydes (PFALds) and n:2 fluorotelomer
aldehydes (FTALds). Both classes are degradation products of known industrial
compounds and environmental contaminants such as fluorotelomer alcohols, iodides,
acrylates, phosphate esters, and other derivatives, as well as hydrofluorocarbons
and hydrochlorofluorocarbons. Prior studies have generally failed to consider the
hydration, and subsequent potential hydrate acidity, of these compounds,
resulting in incomplete and erroneous predictions as to their environmental
behavior. In the current work, DFT calculations suggest that all PFALds will be
dominantly present as the hydrated form in aqueous solution. Both SPARC and DFT
calculations suggest that FTALds will not likely be substantially hydrated in
aquatic systems or in vivo. PFALd hydrates are expected to have pK_a values in the
range of phenols (ca. 9 to 10), whereas n:2 FTALd hydrates are expected to have
pK_a values ca. 2 to 3 units higher (ca. 12 to 13). In order to avoid spurious
modeling predictions and a fundamental misunderstanding of their fate, the
molecular and/or dissociated hydrate forms of PFALds and FTALds need to be
explicitly considered in environmental, toxicological, and waste treatment
investigations. The results of the current study will facilitate a more complete
examination of the environmental fate of PFALds and FTALds.

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LA - eng

PT - Journal Article
 DEP - 20160316
 PL - England
 TA - J Environ Sci Health A Tox Hazard Subst Environ Eng
 JT - Journal of environmental science and health. Part A, Toxic/hazardous substances & environmental engineering
 JID - 9812551
 SB - IM
 OTO - NOTNLM
 OT - Hydration
 OT - fluorotelomer aldehydes
 OT - hydrate acidity
 OT - perfluoroalkyl aldehydes
 EDAT- 2016/03/17 06:00
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 PHST- 2016/03/16 [aheadofprint]
 AID - 10.1080/10934529.2016.1141625 [doi]
 PST - ppublish
 SO - J Environ Sci Health A Tox Hazard Subst Environ Eng. 2016 Jun 6;51(7):579-82.
 doi: 10.1080/10934529.2016.1141625. Epub 2016 Mar 16.

 PMID- 27045622
 OWN - NLM
 STAT- Publisher
 DA - 20160405
 LR - 20160406
 IS - 1873-3336 (Electronic)
 IS - 0304-3894 (Linking)
 VI - 313
 DP - 2016 Mar 29
 TI - Low dose perfluorooctanoate exposure promotes cell proliferation in a human non-tumor liver cell line.
 PG - 18-28
 LID - S0304-3894(16)30301-6 [pii]
 LID - 10.1016/j.jhazmat.2016.03.077 [doi]
 AB - Perfluorooctanoate (PFOA) is a well-known persistent organic pollutant widely found in the environment, wildlife and humans. Medical surveillance and experimental studies have investigated the potential effects of PFOA on human livers, but the hepatotoxicity of PFOA on humans and its underlying mechanism remain to be clarified. We exposed a human liver cell line (HL-7702) to 50muM PFOA for 48h and 96h, and identified 111 significantly differentially expressed proteins by iTRAQ analysis. A total of 46 proteins were related to cell proliferation and apoptosis. Through further analysis of the cell cycle, apoptosis and their related proteins, we found that low doses of PFOA (50-100muM) promoted cell proliferation and numbers by promoting cells from the G1 to S phases, whereas high doses of PFOA (200-400muM) led to reduced HL-7702 cell numbers compared with that of the control mainly due to cell cycle arrest in the

G0/G1 phase. To our knowledge, this is the first report on the promotion of cell cycle progression in human cells following PFOA exposure.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20160329

TA - J Hazard Mater

JT - Journal of hazardous materials

JID - 9422688

OTO - NOTNLM

OT - Cell proliferation

OT - Human cells

OT - PFOA

OT - iTRAQ

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SO - J Hazard Mater. 2016 Mar 29;313:18-28. doi: 10.1016/j.jhazmat.2016.03.077.

PMID- 27016666

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STAT- Publisher

DA - 20160326

LR - 20160327

IS - 1873-3336 (Electronic)

IS - 0304-3894 (Linking)

VI - 312

DP - 2016 Mar 16

TI - Occurrence and distribution of brominated flame retardants and perfluoroalkyl substances in Australian landfill leachate and biosolids.

PG - 55-64

LID - S0304-3894(16)30253-9 [pii]

LID - 10.1016/j.jhazmat.2016.03.031 [doi]

AB - The levels of perfluoroalkyl substances (PFASs), polybrominated diphenyl ethers (PBDEs) and hexabromocyclododecane (HBCDDs) were studied in Australian landfill leachate and biosolids. Leachate was collected from 13 landfill sites and biosolids were collected from 16 wastewater treatment plants (WWTPs), across Australia. Perfluorohexanoate (PFHxA) (12-5700ng/L) was the most abundant investigated persistent, bioaccumulative and toxic (PBT) chemical in leachate. With one exception, mean concentrations of PFASs were higher in leachate of operating landfills compared to closed landfills. Polybrominated diphenyl ethers (PBDEs) and hexabromocyclododecane isomers (HBCDDs) were detected typically at operating landfills in comparatively lower concentrations than the PFASs. Decabromodiphenyl ether (BDE-209) (<0.4-2300ng/g) and perfluorooctanesulfonate (PFOS) (<LOD-380ng/g) were the predominant PBTs detected in biosolids. Using data provided by sites, the volume of leachate discharged to WWTPs for treatment was small (<1% total inflow), and masses of PBTs transferred reached a maximum of 16g/yr (PFHxA). A national estimate of masses of PBTs accumulated in Australian biosolids reached 167kg/yr (BDE-209), a per capita contribution of 7.2+/-7.2mg/yr. Nationally, approximately 59% of biosolids are repurposed and applied to agricultural land. To our knowledge this study presents the first published data of PFASs and HBCDDs in Australian leachate and biosolids.

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LA - ENG
PT - JOURNAL ARTICLE
DEP - 20160316
TA - J Hazard Mater
JT - Journal of hazardous materials
JID - 9422688
OTO - NOTNLM
OT - Biosolids
OT - Hexabromocyclododecane (HBCDD)
OT - Leachate
OT - Perfluoroalkyl substances (PFASs)
OT - Polybrominated diphenyl ethers (PBDE)
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AID - S0304-3894(16)30253-9 [pii]
AID - 10.1016/j.jhazmat.2016.03.031 [doi]
PST - aheadofprint
SO - J Hazard Mater. 2016 Mar 16;312:55-64. doi: 10.1016/j.jhazmat.2016.03.031.

PMID- 26686481
OWN - NLM
STAT- In-Data-Review
DA - 20160109
IS - 1873-3336 (Electronic)
IS - 0304-3894 (Linking)
VI - 305
DP - 2016 Mar 15
TI - Toxicity and bioaccumulation of copper in *Limnodrilus hoffmeisteri* under

different pH values: Impacts of perfluorooctane sulfonate.

PG - 219-28

LID - 10.1016/j.jhazmat.2015.11.048 [doi]

LID - S0304-3894(15)30249-1 [pii]

AB - Aquatic oligochaete *Limnodrilus hoffmeisteri* (*L. hoffmeisteri*) has been commonly used as a lethal and/or sub-lethal toxicological model organism in ecological risk assessments in contaminated water environments. In this study, experiments were conducted to investigate the potential toxic effects of copper (Cu(II)) with or without perfluorooctane sulfonate (PFOS) under different pH values (6.0, 7.0 and 8.0) on LC50, bioaccumulation, and oxidative stress biomarkers in *L. hoffmeisteri* after 3 and 7 days. The LC50 values of Cu(II) decreased with the increasing pH and the addition of PFOS. After each exposure, increasing bioaccumulation of Cu(II) in *L. hoffmeisteri* was observed in the combined exposure treatments, whereas the bioaccumulation of PFOS decreased. Moreover, the activity of superoxide dismutase, the level of glutathione, and the content of malondialdehyde were significantly altered after these exposures, possibly indicating that the bioaccumulation of Cu(II) and PFOS caused adverse effects on antioxidant defenses of *L. hoffmeisteri*. The integrated biomarker response index, indicates that the combined effect was proposed as synergism, which is coincided with the results of toxic unit. Moreover, this work showed that aquatic environment may become more livable when water conditions changed from acidic to near-neutral or alkaline.

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 LA - eng
 PT - Journal Article
 DEP - 20151202
 PL - Netherlands
 TA - J Hazard Mater
 JT - Journal of hazardous materials
 JID - 9422688
 SB - IM
 OTO - NOTNLM
 OT - Bioaccumulation
 OT - Copper
 OT - Different pH values
 OT - Limnodrilus hoffmeisteri
 OT - Oxidative stress
 OT - Perfluorooctane sulfonate
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 AID - 10.1016/j.jhazmat.2015.11.048 [doi]
 PST - ppublish
 SO - J Hazard Mater. 2016 Mar 15;305:219-28. doi: 10.1016/j.jhazmat.2015.11.048. Epub 2015 Dec 2.

 PMID- 26181512
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160106
 LR - 20160204
 IS - 1547-6901 (Electronic)
 IS - 1547-691X (Linking)
 VI - 13
 IP - 2
 DP - 2016 Mar
 TI - Antibody response to booster vaccination with tetanus and diphtheria in adults

exposed to perfluorinated alkylates.

PG - 270-3

LID - 10.3109/1547691X.2015.1067259 [doi]

AB - Recent studies suggest that exposure to perfluorinated alkylate substances (PFASs) may induce immunosuppression in humans and animal models. In this exploratory study, 12 healthy adult volunteers were recruited. With each subject, serum-PFAS concentrations were measured and their antibody responses prospectively followed for 30 days after a booster vaccination with diphtheria and tetanus. The results indicated that serum-PFAS concentrations were positively correlated and positively associated with age and male sex. The specific antibody concentrations in serum were increased from Day 4 to Day 10 post-booster, after which a constant concentration was reached. Serum PFAS concentrations showed significant negative associations with the rate of increase in the antibody responses. Interestingly, this effect was particularly strong for the longer-chain PFASs. All significant associations remained significant after adjustment for sex and age. Although the study involved a small number of subjects, these findings of a PFAS-associated reduction of the early humoral immune response to booster vaccination in healthy adults supported previous findings of PFAS immunosuppression in larger cohorts. Furthermore, the results suggested that cellular mechanisms right after antigen exposure should be investigated more closely to identify possible mechanisms of immunosuppression from PFAS.

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 LA - eng
 GR - R01 ES012199/ES/NIEHS NIH HHS/United States
 PT - Journal Article
 DEP - 20150716
 PL - England
 TA - J Immunotoxicol
 JT - Journal of immunotoxicology
 JID - 101201960
 SB - IM
 PMC - PMC4739630
 MID - NIHMS753623
 OID - NLM: NIHMS753623 [Available on 03/01/17]
 OID - NLM: PMC4739630 [Available on 03/01/17]
 OTO - NOTNLM
 OT - Antibodies
 OT - immunotoxicity
 OT - perfluorinated alkylate substances
 OT - prospective study
 OT - vaccinations
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 MHDA- 2015/07/17 06:00
 CRDT- 2015/07/17 06:00
 PMCR- 2017/03/01 00:00
 PHST- 2015/07/16 [aheadofprint]
 AID - 10.3109/1547691X.2015.1067259 [doi]
 PST - ppublish
 SO - J Immunotoxicol. 2016 Mar;13(2):270-3. doi: 10.3109/1547691X.2015.1067259. Epub
 2015 Jul 16.

 PMID- 25812627
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160106
 IS - 1547-6901 (Electronic)
 IS - 1547-691X (Linking)
 VI - 13
 IP - 2
 DP - 2016 Mar
 TI - Cord blood gene expression supports that prenatal exposure to perfluoroalkyl
 substances causes depressed immune functionality in early childhood.
 PG - 173-80
 LID - 10.3109/1547691X.2015.1029147 [doi]
 AB - Perfluoroalkyl and polyfluoroalkyl substances (PFAS) are a class of synthetic
 compounds that have widespread use in consumer and industrial applications. PFAS
 are considered environmental pollutants that have various toxic properties,

including effects on the immune system. Recent human studies indicate that prenatal exposure to PFAS leads to suppressed immune responses in early childhood. In this study, data from the Norwegian BraMat cohort was used to investigate transcriptomics profiles in neonatal cord blood and their association with maternal PFAS exposure, anti-rubella antibody levels at 3 years of age and the number of common cold episodes until 3 years. Genes associated with PFAS exposure showed enrichment for immunological and developmental functions. The analyses identified a toxicogenomics profile of 52 PFAS exposure-associated genes that were in common with genes associated with rubella titers and/or common cold episodes. This gene set contains several immunomodulatory genes (CYTL1, IL27) as well as other immune-associated genes (e.g. EMR4P, SHC4, ADORA2A). In addition, this study identified PPARD as a PFAS toxicogenomics marker. These markers can serve as the basis for further mechanistic or epidemiological studies. This study provides a transcriptomics connection between prenatal PFAS exposure and impaired immune function in early childhood and supports current views on PPAR- and NF-kappaB-mediated modes of action. The findings add to the available evidence that PFAS exposure is immunotoxic in humans and support regulatory policies to phase out these substances.

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LA - eng
PT - Journal Article
DEP - 20150327
PL - England
TA - J Immunotoxicol
JT - Journal of immunotoxicology
JID - 101201960
SB - IM
OTO - NOTNLM
OT - Immunotoxicity
OT - perfluoroalkyl carboxylic acids
OT - perfluoroalkyl substances
OT - perfluoroalkyl sulfonic acids
OT - prenatal exposure
OT - toxicogenomics
EDAT- 2015/03/31 06:00
MHDA- 2015/03/31 06:00
CRDT- 2015/03/28 06:00
PHST- 2015/03/27 [aheadofprint]
AID - 10.3109/1547691X.2015.1029147 [doi]
PST - ppublish
SO - J Immunotoxicol. 2016 Mar;13(2):173-80. doi: 10.3109/1547691X.2015.1029147. Epub 2015 Mar 27.

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DA - 20160318

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IS - 1708-8267 (Electronic)

IS - 1081-5589 (Linking)

DP - 2016 Mar 17

TI - Patent foramen ovale (PFO), stroke and pregnancy.

LID - jim-2016-000103 [pii]

AB - Patent foramen ovale (PFO)-related stroke is increasingly recognized as an important etiology of ischemic embolic stroke-accounting for up to 50% of strokes previously considered 'cryptogenic' or with an unknown mechanism. As a 'back door to the brain,' PFO can allow venous clots to enter arterial circulation via interatrial right-to-left shunting, potentially resulting in ischemic stroke. We observe that clinically, PFO-related stroke affects women of childbearing age, and that pregnancy-owing to major changes in hemocoagulative, hormonal, and cardiovascular parameters-can enhance stroke risks. However, no systematic study has been performed and little is known regarding complications, pregnancy outcomes and treatment for PFO-related stroke during pregnancy. To identify and characterize the complications and clinical outcomes related to PFOs during pregnancy, we performed a literature review and analysis from all reported cases of pregnancy with PFO-related complications in the medical literature from 1970 to 2015. We find that during pregnancy and post-partum, PFO is associated with

complications affecting multiple organs, including the brain, heart and lung. The three principal complications reported are stroke, pulmonary emboli and myocardial infarction. In contrast to other pregnancy-related stroke etiologies, which peak during later pregnancy and postpartum, PFO-related stroke peaks during early pregnancy (first and second trimester-60%), and most patients had good neurological outcome (77%). In patients with PFO with recurrent stroke during pregnancy, additional key factors include high-risk PFO morphology (atrial septal aneurysm), larger right-to-left shunt, multiple gestation and concurrent hypercoagulability. Compared to strokes of other etiologies during pregnancy, most PFO stroke patients experienced uneventful delivery (93%) of healthy babies with a good clinical outcome. We conclude with recommended clinical treatment strategies for pregnant patients with PFO suggested by the data from these cases, and the clinical experience of our Cardio-Neurology Clinic.

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 LA - ENG
 PT - REVIEW
 PT - JOURNAL ARTICLE
 DEP - 20160317
 TA - J Investig Med
 JT - Journal of investigative medicine : the official publication of the American
 Federation for Clinical Research
 JID - 9501229
 OTO - NOTNLM
 OT - Myocardial Infarction
 OT - Pregnancy
 OT - Pulmonary Embolism
 OT - Stroke
 EDAT- 2016/03/19 06:00
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 AID - jim-2016-000103 [pii]
 AID - 10.1136/jim-2016-000103 [doi]
 PST - aheadofprint
 SO - J Investig Med. 2016 Mar 17. pii: jim-2016-000103.

 PMID- 26980724
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160415
 IS - 1520-6904 (Electronic)
 IS - 0022-3263 (Linking)
 VI - 81
 IP - 8
 DP - 2016 Apr 15
 TI - Cu-Catalyzed Multicomponent Reaction of Styrenes, Perfluoroalkyl Halide, Alcohol,
 and tert-Butyl Hydroperoxide: One-Pot Synthesis of
 (Z)-beta-Alkoxyperfluoroalkenone.
 PG - 3103-11
 LID - 10.1021/acs.joc.5b02664 [doi]
 AB - An efficient synthesis of Z-perfluoroalkyl-substituted enones by a multicomponent
 reaction strategy has been described. A variety of elusive perfluoroalkylated
 enones are furnished under mild reaction conditions in good yields with unique
 chemo- and stereoselectivity. A sequence of radical-mediated Kornblum-DeLaMare
 reaction, Michael addition, and HF elimination is proposed for the mechanism.
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LA - eng
PT - Journal Article
DEP - 20160325
PL - United States
TA - J Org Chem
JT - The Journal of organic chemistry
JID - 2985193R
SB - IM

EDAT- 2016/03/17 06:00
MHDA- 2016/03/17 06:00
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PHST- 2016/03/25 [aheadofprint]
AID - 10.1021/acs.joc.5b02664 [doi]
PST - ppublish
SO - J Org Chem. 2016 Apr 15;81(8):3103-11. doi: 10.1021/acs.joc.5b02664. Epub 2016 Mar 25.

PMID- 27031195
OWN - NLM
STAT- Publisher
DA - 20160331
LR - 20160401
IS - 1873-2682 (Electronic)
IS - 1011-1344 (Linking)
VI - 159
DP - 2016 Mar 18
TI - Effects of perfluorooctane sulfonate on the conformation and activity of bovine serum albumin.
PG - 66-73
LID - S1011-1344(16)30057-4 [pii]
LID - 10.1016/j.jphotobiol.2016.03.024 [doi]
AB - Perfluorooctane sulfonate (PFOS) is among the most prominent contaminants in human serum and has been reported to possess potential toxicity to the human body. In this study, the effects of PFOS on the conformation and activity of bovine serum albumin (BSA) were investigated in vitro. The results indicated that the binding interaction of PFOS with BSA destroyed the tertiary and secondary structures of protein with the loss of alpha-helix structure and the increasing of hydrophobic microenvironment of the Trp or Tyr residues. During the thermal denaturation protein, PFOS increases the protein stability of BSA. The proportion of alpha-helix decreased on increasing the PFOS concentration and the microenvironment of the Trp or Tyr residues becomes more hydrophobic. The results from molecular modeling indicated that BSA had not only one possible binding site to bind with PFOS by the polar interaction, hydrogen bonds and hydrophobic forces. In addition, the BSA relative activities were decreased with the increase of PFOS concentration. Such loss of BSA activity in the presence of PFOS indicated that one of the binding sites in BSA is located in subdomain IIIA, which is in good agreement with the fluorescence spectroscopic experiments and molecular modeling results. This study offers a comprehensive picture of the interactions of PFOS with serum albumin and provides insights into the toxicological effect of perfluoroalkylated substances.
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 LA - ENG
 PT - JOURNAL ARTICLE
 DEP - 20160318
 TA - J Photochem Photobiol B
 JT - Journal of photochemistry and photobiology. B, Biology
 JID - 8804966
 OTO - NOTNLM
 OT - Denaturation
 OT - Perfluorooctane sulfonate
 OT - Secondary structure
 OT - Serum albumin
 OT - Toxicological evaluation
 EDAT- 2016/04/01 06:00
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 PHST- 2016/03/15 [revised]
 PHST- 2016/03/15 [accepted]
 AID - S1011-1344(16)30057-4 [pii]
 AID - 10.1016/j.jphotobiol.2016.03.024 [doi]
 PST - aheadofprint
 SO - J Photochem Photobiol B. 2016 Mar 18;159:66-73. doi:
 10.1016/j.jphotobiol.2016.03.024.

 PMID- 26848611
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160310
 IS - 1520-5207 (Electronic)
 IS - 1520-5207 (Linking)
 VI - 120
 IP - 9
 DP - 2016 Mar 10
 TI - Characterization of Adsorbed Molecular Water on the Surface of a Stretched Polytetrafluoroethylene Tape Analyzed by (1)H NMR.

PG - 2538-43
LID - 10.1021/acs.jpcb.5b11276 [doi]
AB - A single molecule often exhibits a largely different material character from a bulk matter. Although a perfluoroalkyl (Rf) compound is a representative one, many interests have mostly been devoted to the bulk character only thus far, leaving the single molecular character unclear. Recently, a new theoretical framework, stratified dipole-arrays (SDA) theory, has appeared for comprehensive understanding of Rf compounds in terms of both single and bulk systems. On this theory, a mechanically stretched polytetrafluoroethylene (PTFE) is expected to exhibit a single-molecular character having dipole-driven properties, which should attract molecular water. In the present study, a stretched PTFE tape is revealed to attract molecular water (not water droplet) in fact, and the adsorbed water molecules are highly restricted in motion by the dipole-dipole interaction studied by using (1)H NMR, which agrees with the prediction by the SDA theory.
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LA - eng
PT - Journal Article
DEP - 20160218
PL - United States
TA - J Phys Chem B
JT - The journal of physical chemistry. B
JID - 101157530
SB - IM
EDAT- 2016/02/06 06:00
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AID - 10.1021/acs.jpcb.5b11276 [doi]
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SO - J Phys Chem B. 2016 Mar 10;120(9):2538-43. doi: 10.1021/acs.jpcb.5b11276. Epub 2016 Feb 18.

PMID- 26982570
OWN - NLM
STAT- In-Data-Review
DA - 20160407
IS - 1520-5207 (Electronic)
IS - 1520-5207 (Linking)
VI - 120
IP - 13

DP - 2016 Apr 7
TI - PFC and Triglyme for Li-Air Batteries: A Molecular Dynamics Study.
PG - 3370-7
LID - 10.1021/acs.jpcc.5b12075 [doi]
AB - In this work, we present an all-atom molecular dynamics (MD) study of triglyme and perfluorinated carbons (PFCs) using classical atomistic force fields. Triglyme is a typical solvent used in nonaqueous Li-air battery cells. PFCs were recently reported to increase oxygen availability in such cells. We show that O₂ diffusion in two specific PFC molecules (C₆F₁₄ and C₈F₁₈) is significantly faster than in triglyme. Furthermore, by starting with two very different initial configurations for our MD simulation, we demonstrate that C₈F₁₈ and triglyme do not mix. The mutual solubility of these molecules is evaluated both theoretically and experimentally, and a qualitative agreement is found. Finally, we show that the solubility of O₂ in C₈F₁₈ is considerably higher than in triglyme. The significance of these results to Li-air batteries is discussed.
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LA - eng
PT - Journal Article
DEP - 20160324
PL - United States
TA - J Phys Chem B
JT - The journal of physical chemistry. B
JID - 101157530
SB - IM
EDAT- 2016/03/17 06:00
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PHST- 2016/03/24 [aheadofprint]
AID - 10.1021/acs.jpcc.5b12075 [doi]
PST - ppublish
SO - J Phys Chem B. 2016 Apr 7;120(13):3370-7. doi: 10.1021/acs.jpcc.5b12075. Epub 2016 Mar 24.

PMID- 26963137
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160407
 IS - 1520-5207 (Electronic)
 IS - 1520-5207 (Linking)
 VI - 120
 IP - 13
 DP - 2016 Apr 7
 TI - Mapping and Tuning the Fluorescence of Perfluorinated Polyanilines Synthesized through Liquid-Liquid Interfaces.
 PG - 3441-54
 LID - 10.1021/acs.jpcb.6b00739 [doi]
 AB - A series of light-emitting perfluorinated polyanilines were synthesized by the oxidative polymerization of 3-perfluorooctyl aniline through a variety of aqueous/organic interfaces. According to the interfacial tension between the two solvents (the organic being chloroform, dichloromethane, perfluorinated ether, toluene, or o-dichlorobenzene), we obtain distinctive classes of materials based on the crystal packing, protonation, and oxidation state of the polymeric chains. We distinguish between soluble fractions with a distinctive, strong, and red-shifted photoluminescence pattern and an insoluble precipitate which can be subsequently solubilized in a mixture of acetone and toluene. The emission maximum for the insoluble fraction is located in the ultraviolet or blue region with a small Stokes shift; maxima for the soluble counterparts are in the green to yellow region. The soluble derivatives demonstrate a significantly smaller band gap compared to the monomer and large Stokes shifts up to 163 nm; the emission maximum for the most red-shifted emission was located at $\lambda_{em} = 548$ nm. Their redox activity toward silver nanoparticles, their sensor reactivity with organic acid and bases, and the subsequent changes in the optical properties were demonstrated and the structure of the materials was evaluated with NMR, X-ray diffraction, and FTIR/Raman spectroscopy.
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 LA - eng
 PT - Journal Article
 DEP - 20160323
 PL - United States
 TA - J Phys Chem B
 JT - The journal of physical chemistry. B
 JID - 101157530

SB - IM
 EDAT- 2016/03/11 06:00
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 PHST- 2016/03/23 [aheadofprint]
 AID - 10.1021/acs.jpcc.6b00739 [doi]
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 SO - J Phys Chem B. 2016 Apr 7;120(13):3441-54. doi: 10.1021/acs.jpcc.6b00739. Epub 2016 Mar 23.

 PMID- 26785284
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160328
 IS - 1876-7737 (Electronic)
 VI - 137
 DP - 2016 Mar 30
 TI - Using a novel "Integrated Biomarker Proteomic" index to assess the effects of freshwater pollutants in European eel peripheral blood mononuclear cells.
 PG - 83-96
 LID - 10.1016/j.jprot.2016.01.007 [doi]
 LID - S1874-3919(16)30009-4 [pii]
 AB - Using proteomic data as biomarkers of environmental pollution has the potential to be of a great interest in ecological risk assessment as they constitute early warning indicators of ecologically relevant effects on biological systems. To develop such specific and sensitive biomarkers, the use of a set of proteins is required and the identification of protein expression signatures (PES) may reflect the exposure to specific classes of pollutants. Using 2D-DIGE (Differential in Gel Electrophoresis) methodology, this study aimed at identifying specific PES on European eel (*Anguilla anguilla*) peripheral blood mononuclear cells (PBMC) after 48h in vitro exposure to two sublethal concentrations of dichlorodiphenyltrichloroethane (p,p'-DDT) (10µg/L and 1µg/L) or cadmium (Cd) (1µg/L and 100µg/L). The present results have been supplemented with data of a first in vitro study on cells exposed to perfluorooctane sulfonate (PFOS) (10µg/L and 1µg/L). A total of thirty-four protein spots, belonging to 18 different identified proteins found in all conditions, have been selected as possible biomarkers to develop a synthetic Integrated Biomarker Proteomic (IBP) index. IBP follows a dose-response relationship with higher values at the highest tested concentration for each pollutant (Cd: 9.96; DDT: 7.44; PFOS: 7.94) compared to the lowest tested concentration (Cd: 3.81; DDT: 2.91; PFOS: 2.06). In a second step, star plot graphs have been applied to proteomic data in order to allow visual integration of a set of early warning responses measured with protein biomarkers. Such star plots permit to discriminate the type of pollutant inducing a proteomic response. We conclude that using IBP is relevant in environmental risk assessment, giving to this index the potential to be applied as a global index of proteome alteration in endangered species such as the European eel. BIOLOGICAL SIGNIFICANCE: In this study, 34 protein spots have been selected as possible biomarkers to develop a synthetic Integrated Biomarker

Proteomic index (IBP). Results show that IBP follows a dose-response relationship with higher values at the highest tested concentration for each pollutant compared to the lowest tested concentration. Star plot graphs have also been applied to proteomic data in order to allow visual integration of a set of early warning responses measured with protein biomarkers. Such star plots permit to discriminate the type of pollutant inducing a proteomic response. IBP is relevant in environmental risk assessment, giving to this index the potential to be applied as a global index of proteome alteration in endangered species such as the European eel.

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LA - eng

PT - Journal Article

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PL - Netherlands

TA - J Proteomics

JT - Journal of proteomics

JID - 101475056

SB - IM

OTO - NOTNLM

OT - Anguilla anguilla

OT - Biomarkers

OT - Cd

OT - DDT

OT - Environmental risk assessment

OT - Integrated Biomarker Proteomic index

OT - Proteomics

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 AID - 10.1016/j.jprot.2016.01.007 [doi]
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 SO - J Proteomics. 2016 Mar 30;137:83-96. doi: 10.1016/j.jprot.2016.01.007. Epub 2016 Jan 16.

 PMID- 26766498
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160331
 IS - 1615-9314 (Electronic)
 IS - 1615-9306 (Linking)
 VI - 39
 IP - 6
 DP - 2016 Mar
 TI - Evaluation of the dual retention properties of stationary phases based on silica hydride: Perfluorinated bonded material.
 PG - 1050-5
 LID - 10.1002/jssc.201501241 [doi]
 AB - The synthesis of a new perfluorinated stationary phase based on silica hydride using a hydrosilation reaction was investigated. The material was characterized by elemental analysis, diffuse reflectance infrared Fourier transform spectroscopy and (13) C cross-polarization magic-angle spinning NMR spectroscopy. The retention properties of this new material were tested in the reversed-phase and normal-phase mode. Variable buffer strength experiments at two pH conditions for selected polar compounds were used to compare the new phase to hydrophilic interaction liquid chromatography retention. These results and previous data reported in the literature were used to postulate differences in the retention mechanism between hydrophilic interaction liquid chromatography and silica hydride-based stationary phases.
 CI - (c) 2016 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.
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 LA - eng
 PT - Journal Article
 DEP - 20160217

PL - Germany
TA - J Sep Sci
JT - Journal of separation science
JID - 101088554
SB - IM
OTO - NOTNLM
OT - Aqueous normal-phase chromatography
OT - Retention mechanisms
OT - Solvent composition studies
OT - Spectroscopic characterization
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PHST- 2016/02/17 [aheadofprint]
AID - 10.1002/jssc.201501241 [doi]
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OWN - NLM

STAT- Publisher

DA - 20160319

LR - 20160320

IS - 0148-6071 (Electronic)

IS - 0148-6071 (Linking)

DP - 2016 Mar 18

TI - A Comparison of Fish Oil Sources for Parenteral Lipid Emulsions in a Murine Model.

LID - 0148607116640275 [pii]

AB - BACKGROUND: Fat emulsions are important components of parenteral nutrition (PN). Fish oil (FO) emulsions reverse cholestasis in PN-associated liver disease. There are 2 FO monographs. One is "FO; rich in omega-3 fatty acids" (NFO). The other, "omega-3 acids," (PFO), is enriched in omega-3 fatty acids, particularly eicosapentaenoic acid (EPA) and docosahexaenoic acid (DHA). The purpose of this study is to compare the effects of 20% NFO and PFO emulsions produced in the laboratory in a murine model. METHODS: Emulsions were compounded containing different oils: soybean oil (SO), NFO, and two PFOs differing in percentage of fatty acids as triglycerides (PFO66 and PFO90). Chow-fed mice received saline, one of the above emulsions, or a commercial FO (OM) intravenously (2.4 g/kg/day) for 19 days. On day 19, animals were euthanized. Livers, spleens, and lungs were procured for histologic analysis. RESULTS: OM, SO, NFO, and PFO90 were well-tolerated clinically. PFO66 resulted in tachypnea and lethargy for ~1 minute following injections. At euthanasia, PFO66 and PFO90 groups had organomegaly. Histologically, these groups had splenic and hepatic fat-laden macrophages, and lungs had scattered fat deposits. Other groups had normal organs. CONCLUSIONS:

PFO emulsions present an attractive possibility for improving inflammation in PN-dependent patients by concentrating anti-inflammatory EPA and DHA. However, 20% PFO emulsions were poorly tolerated and precipitated adverse end organ sequelae, suggesting that they may not be safe. Development of novel manufacturing methods may achieve safe 20% PFO parenteral emulsions, but by established formulation methods, these emulsions were clinically suboptimal despite meeting pharmacopeial standards.

CI - (c) 2016 American Society for Parenteral and Enteral Nutrition.

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LA - ENG

PT - JOURNAL ARTICLE
 DEP - 20160318
 TA - JPEN J Parenter Enteral Nutr
 JT - JPEN. Journal of parenteral and enteral nutrition
 JID - 7804134
 OTO - NOTNLM
 OT - USP 729
 OT - fish oil
 OT - intestinal failure
 OT - parenteral lipid emulsions
 OT - parenteral nutrition-associated liver disease
 EDAT- 2016/03/20 06:00
 MHDA- 2016/03/20 06:00
 CRDT- 2016/03/20 06:00
 AID - 0148607116640275 [pii]
 AID - 10.1177/0148607116640275 [doi]
 PST - aheadofprint
 SO - JPEN J Parenter Enteral Nutr. 2016 Mar 18. pii: 0148607116640275.

 PMID- 26881998
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160315
 IS - 1520-5827 (Electronic)
 IS - 0743-7463 (Linking)
 VI - 32
 IP - 10
 DP - 2016 Mar 15
 TI - Perfluorinated Alcohols Induce Complex Coacervation in Mixed Surfactants.
 PG - 2321-30
 LID - 10.1021/acs.langmuir.5b04701 [doi]
 AB - Recently, we reported a unique and nearly ubiquitous phenomenon of inducing simple and complex coacervation in solutions of a broad variety of individual and mixed amphiphiles and over a wide range of concentrations and mole fractions. This paper describes a novel type of biphasic separation in aqueous solutions of mixed cationic-anionic (catanionic) surfactants induced by hexafluoroisopropanol (HFIP). The test cases included mixtures of cetyltrimethylammonium bromide (CTAB) and sodium dodecyl sulfate (SDS) (surfactants with different carbon chain lengths) as well as dodecyltrimethylammonium bromide (DTAB) with SDS (surfactants with the same carbon chain lengths). The CTAB-SDS-HFIP coacervate systems can be produced at many different mole ratios of surfactant, but DTAB-SDS-HFIP formed only coacervates at equimolar (1:1) mole ratios of DTAB and SDS. The phase-transition behavior of both systems was studied over a wide range of surfactant and HFIP concentrations at the stoichiometric (1:1) mole ratio of cationic/anionic surfactants. The chemical compositions of each of the two phases (aqueous-rich and coacervate phases) were studied with regard to the concentrations of HFIP, water, and individual surfactants. It is revealed that the surfactant-rich phase (coacervate phase) contains a large percentage of

fluoroalcohol relative to the aqueous phase and is enriched in both surfactants but contains a small percentage of water. Surprisingly, the concentration of water in the coacervate phase increases as the total HFIP concentration is increased while the concentration of HFIP in the coacervate phase remains relatively constant, which means a larger amount of water associated with HFIP molecules is extracted into the coacervate phase, which results in the growth of the phase. The volume of the coacervate phase increases with an increase in surfactant concentration and total HFIP %. The coacervate phase is highly enriched in the two amphiphilic ions (DTA(+) and DS(-)) whereas the two counterions (Br(-) and Na(+)) primarily reside in the aqueous-rich phase. The results suggest the formation of a catanionic complex in the coacervate phase through ion pairing with a concomitant release of the surfactant counterions (Na(+) and Br(-)) into the aqueous-rich phase. Finally, the fluorocarbon alcohol systems are contrasted with the effects of aliphatic alcohols in the mixed catanionic surfactant systems. Isopropanol does not have the same interactions as HFIP with respect to solubilization, aggregation, and phase separation of the oppositely charged surfactants.

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LA - eng

PT - Journal Article

DEP - 20160229

PL - United States

TA - Langmuir

JT - Langmuir : the ACS journal of surfaces and colloids

JID - 9882736

SB - IM

EDAT- 2016/02/18 06:00

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PHST- 2016/02/29 [aheadofprint]

AID - 10.1021/acs.langmuir.5b04701 [doi]

PST - ppublish

SO - Langmuir. 2016 Mar 15;32(10):2321-30. doi: 10.1021/acs.langmuir.5b04701. Epub 2016 Feb 29.

PMID- 26626141

OWN - NLM
STAT- In-Data-Review
DA - 20160206
IS - 1097-458X (Electronic)
IS - 0749-1581 (Linking)
VI - 54
IP - 3
DP - 2016 Mar
TI - Monitoring oil displacement processes with k-t accelerated spin echo SPI.
PG - 197-204
LID - 10.1002/mrc.4362 [doi]
AB - Magnetic resonance imaging (MRI) is a robust tool to monitor oil displacement processes in porous media. Conventional MRI measurement times can be lengthy, which hinders monitoring time-dependent displacements. Knowledge of the oil and water microscopic distribution is important because their pore scale behavior reflects the oil trapping mechanisms. The oil and water pore scale distribution is reflected in the magnetic resonance T2 signal lifetime distribution. In this work, a pure phase-encoding MRI technique, spin echo SPI (SE-SPI), was employed to monitor oil displacement during water flooding and polymer flooding. A k-t acceleration method, with low-rank matrix completion, was employed to improve the temporal resolution of the SE-SPI MRI measurements. Comparison to conventional SE-SPI T2 mapping measurements revealed that the k-t accelerated measurement was more sensitive and provided higher-quality results. It was demonstrated that the k-t acceleration decreased the average measurement time from 66.7 to 20.3 min in this work. A perfluorinated oil, containing no (1) H, and H2 O brine were employed to distinguish oil and water phases in model flooding experiments. High-quality 1D water saturation profiles were acquired from the k-t accelerated SE-SPI measurements. Spatially and temporally resolved T2 distributions were extracted from the profile data. The shift in the (1) H T2 distribution of water in the pore space to longer lifetimes during water flooding and polymer flooding is consistent with increased water content in the pore space. Copyright (c) 2015 John Wiley & Sons, Ltd.
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 LA - eng
 PT - Journal Article
 DEP - 20151202
 PL - England
 TA - Magn Reson Chem
 JT - Magnetic resonance in chemistry : MRC
 JID - 9882600
 SB - IM
 OTO - NOTNLM
 OT - 1H
 OT - MRI
 OT - T2 distribution
 OT - enhanced oil recovery
 OT - k-t SE-SPI
 OT - oil displacement
 OT - pore scale fluid behavior
 OT - water saturation profile
 EDAT- 2015/12/03 06:00
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 PHST- 2015/08/31 [revised]
 PHST- 2015/09/03 [accepted]
 PHST- 2015/12/02 [aheadofprint]
 AID - 10.1002/mrc.4362 [doi]
 PST - ppublish
 SO - Magn Reson Chem. 2016 Mar;54(3):197-204. doi: 10.1002/mrc.4362. Epub 2015 Dec 2.

 PMID- 26794494
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160129
 IS - 1879-0291 (Electronic)
 IS - 0141-1136 (Linking)
 VI - 114
 DP - 2016 Mar
 TI - Transcriptomic analysis of bottlenose dolphin (*Tursiops truncatus*) skin biopsies
 to assess the effects of emerging contaminants.
 PG - 74-9
 LID - 10.1016/j.marenvres.2016.01.002 [doi]
 LID - S0141-1136(16)30002-2 [pii]
 AB - Chemicals discovered in water at levels that may be significantly different than
 expected are referred to as contaminants of emerging concern (CECs) because the
 risk to environmental health posed by their occurrence/frequency is still
 unknown. The worldwide distributed compounds perfluorooctanoic acid (PFOA) and

bisphenol A (BPA) may fall into this category due to effects on endocrine receptors. We applied an ex vivo assay using small slices of bioptic skin from the bottlenose dolphin, *Tursiops truncatus*, cultured and treated for 24 h with different PFOA or BPA concentrations to analyze global gene expression. RNA was labeled and hybridized to a species-specific oligomicroarray. The skin transcriptome held information on the contaminant exposure, potentially predictive about long-term effects on health, being the genes affected involved in immunity modulation, response to stress, lipid homeostasis, and development. The transcriptomic signature of dolphin skin could be therefore relevant as classifier for a specific contaminant.

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LA - eng

PT - Journal Article

DEP - 20160109

PL - England

TA - Mar Environ Res

JT - Marine environmental research

JID - 9882895

SB - IM

OTO - NOTNLM

OT - Biomarkers

OT - Bottlenose dolphin

OT - Emerging contaminants

OT - Ocean health

OT - Transcriptome
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PHST- 2015/12/22 [revised]
PHST- 2016/01/07 [accepted]
PHST- 2016/01/09 [aheadofprint]
AID - S0141-1136(16)30002-2 [pii]
AID - 10.1016/j.marenvres.2016.01.002 [doi]
PST - ppublish
SO - Mar Environ Res. 2016 Mar;114:74-9. doi: 10.1016/j.marenvres.2016.01.002. Epub 2016 Jan 9.

PMID- 26948293
OWN - NLM
STAT- In-Data-Review
DA - 20160425
IS - 1879-3363 (Electronic)
IS - 0025-326X (Linking)
VI - 105
IP - 1
DP - 2016 Apr 15
TI - Perfluoroalkylated substances (PFASs) and legacy persistent organic pollutants (POPs) in halibut and shrimp from coastal areas in the far north of Norway: Small survey of important dietary foodstuffs for coastal communities.

PG - 81-7
LID - 10.1016/j.marpolbul.2016.02.053 [doi]
LID - S0025-326X(16)30109-6 [pii]
AB - Halibut (*Hippoglossus hippoglossus*) and shrimps (*Pandalus borealis*) are regular foodstuffs for communities in northern Norway and important species for the coastal fishing industry. This is the first study to present a comprehensive overview of the contaminant status of these species, with emphasis on unregulated perfluoroalkylated substances (PFAS). The contaminant concentrations were low and within tolerable levels for human dietary exposure. Median Sigmapolychlorinated biphenyls (PCB) were 4.9 and 2.5ng/g ww for halibut and unpeeled shrimps, respectively. Concentrations of perfluorooctane sulfonate (PFOS) - the most abundant PFASs - were 0.9 and 2.7ng/g ww in halibut and shrimp, respectively. The halibut fillets were dominated by PCBs, which contributed to 50% of the total POPs load, followed by SigmaDDTs; 26% and PFASs (18%), whereas shrimps were dominated by PFASs (74%). SigmaPBDEs (polybrominated diphenyl ethers) contributed to 1-4% of the total POP load. Local sources are not contributing significantly to the contaminant burden in these species.

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LA - eng

PT - Journal Article

DEP - 20160302

PL - England

TA - Mar Pollut Bull

JT - Marine pollution bulletin

JID - 0260231

SB - IM

OTO - NOTNLM

OT - Arctic

OT - Fish

OT - PBDE

OT - PCB

OT - PFCA

OT - PFOS

EDAT- 2016/03/08 06:00

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PHST- 2016/02/12 [revised]

PHST- 2016/02/19 [accepted]

PHST- 2016/03/02 [aheadofprint]

AID - S0025-326X(16)30109-6 [pii]

AID - 10.1016/j.marpolbul.2016.02.053 [doi]

PST - ppublish

SO - Mar Pollut Bull. 2016 Apr 15;105(1):81-7. doi: 10.1016/j.marpolbul.2016.02.053.
Epub 2016 Mar 2.

PMID- 26978428
OWN - NLM
STAT- In-Data-Review
DA - 20160330
IS - 1477-0539 (Electronic)
IS - 1477-0520 (Linking)
VI - 14
IP - 14
DP - 2016 Apr 14
TI - Maltotriose-conjugation to a fluorinated chlorin derivative generating a PDT
photosensitizer with improved water-solubility.
PG - 3608-13
LID - 10.1039/c6ob00276e [doi]
AB - Photoactive molecules with the frameworks of chlorin and/or porphyrin possessing
four perfluorinated aromatic rings were conjugated with maltotriose (Mal3) via
the nucleophilic aromatic substitution reaction and subsequent deprotection
reaction of the oligosaccharide moieties. The resulting
oligosaccharide-conjugated molecules are ultimately improved as compared to the
previously reported monosaccharide-counterparts in terms of water-solubility. In
particular, a water-soluble chlorin derivative surrounded by four Mal3 molecules
showed an excellent biocompatibility, strong photoabsorption in the longer
wavelength regions, and a very high photocytotoxicity. Thus, the present
synthetic route combined with the use of an oligosaccharide was shown to be a
straightforward strategy to develop a third generation photosensitizer for
photodynamic therapy (PDT).
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FAU - Kikuchi, Jun-Ichi
AU - Kikuchi J
FAU - Yano, Shigenobu
AU - Yano S
LA - eng
PT - Journal Article
DEP - 20160315
PL - England
TA - Org Biomol Chem
JT - Organic & biomolecular chemistry
JID - 101154995
SB - IM
EDAT- 2016/03/16 06:00
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PHST- 2016/03/15 [aheadofprint]
PHST- 2016/03/30 [epublish]
AID - 10.1039/c6ob00276e [doi]
PST - ppublish
SO - Org Biomol Chem. 2016 Apr 14;14(14):3608-13. doi: 10.1039/c6ob00276e. Epub 2016 Mar 15.

PMID- 26492286
OWN - NLM
STAT- In-Data-Review
DA - 20160318
LR - 20160318
IS - 1530-0447 (Electronic)
IS - 0031-3998 (Linking)
VI - 79
IP - 2
DP - 2016 Mar
TI - Perfluoroalkyl and polyfluoroalkyl substances and indicators of immune function in children aged 12-19 y: National Health and Nutrition Examination Survey.
PG - 348-57
LID - 10.1038/pr.2015.213 [doi]
AB - BACKGROUND: Perfluoroalkyl and polyfluoroalkyl substances (PFAS) are immunotoxic in laboratory studies. Human studies of immune effects are inconsistent. Using the US National Health and Nutrition Examination Survey (NHANES), we examined PFAS serum concentration and indicators of prevalent immune function among 12-19-y-old children. METHODS: In this cross-sectional study, we examined PFAS serum concentration in relation to measles, mumps, and rubella antibody concentrations in NHANES 1999-2000 and 2003-2004 (n = 1,191) and to allergic

conditions and allergic sensitization in NHANES 2005-2006 (n = 640). RESULTS: In adjusted, survey-weighted models, a doubling of perfluorooctane sulfonate (PFOS) concentration among seropositive children was associated with a 13.3% (95% confidence interval (CI): -19.9, -6.2) decrease in rubella antibody concentration and a 5.9% decrease in mumps antibody concentration (95% CI: -9.9, -1.6). We observed no adverse association between exposure and current allergic conditions, including asthma. Children with higher PFOS concentration were less likely to be sensitized to any allergen (odds ratio (OR): 0.74; 95% CI: 0.58, 0.95).

CONCLUSION: Increased exposure to several PFAS was associated with lower levels to mumps and rubella antibody concentrations, especially among seropositive individuals. These lower antibody concentrations may indicate a less robust response to vaccination or greater waning of vaccine-derived immunity over time.

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LA - eng

GR - K01 ES019156/ES/NIEHS NIH HHS/United States

GR - P30 ES023515/ES/NIEHS NIH HHS/United States

PT - Journal Article

DEP - 20151022

PL - United States

TA - Pediatr Res

JT - Pediatric research

JID - 0100714

SB - IM

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AID - pr2015213 [pii]
 AID - 10.1038/pr.2015.213 [doi]
 PST - ppublish
 SO - Pediatr Res. 2016 Mar;79(2):348-57. doi: 10.1038/pr.2015.213. Epub 2015 Oct 22.

 PMID- 26992685
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160319
 IS - 1532-3102 (Electronic)
 IS - 0143-4004 (Linking)
 VI - 39
 DP - 2016 Mar
 TI - In utero perfluorooctane sulfonate exposure causes low body weights of fetal rats: A mechanism study.
 PG - 125-33
 LID - 10.1016/j.placenta.2016.01.010 [doi]
 LID - S0143-4004(16)30010-8 [pii]
 AB - OBJECTIVES: The objective of the present study is to investigate the mechanism of perfluorooctane sulfonate-induced low body weight of fetus by analysis of glucocorticoid metabolizing enzyme 11beta-hydroxysteroid dehydrogenase 2 and gene expression profiling of the placenta after in utero PFOS exposure. STUDY DESIGN: Pregnant Sprague-Dawley dams were gavaged with 0, 5, and 20 mg/kg body weight PFOS daily from gestational day 12-18. On gestational day 18, pregnant dams were euthanized, placentas, and fetuses were collected. MAIN OUTCOME MEASURES: Body weights of fetuses and placentas were measured, the corticosterone levels in fetal serum, and 11beta-hydroxysteroid dehydrogenase 2 as well as the placental gene profiling were analyzed. RESULTS: 20 mg/kg PFOS significantly reduced fetal body weight and placental weight. Both 5 and 20 mg/kg PFOS increased fetal serum corticosterone levels. PFOS potently inhibited placental 11beta-hydroxysteroid dehydrogenase 2 activity. Of 21,910 genes, 45 genes were significantly downregulated ≥ 2 fold by 20 mg/kg PFOS, including extracellular matrix (Slpi and Pil6), growth factors and hormones (Trh and Pdf), ion transporters (Aqp1, Sl00a4, and Abpl), signal transducers (Kap and Ampd3), and structural constituents (A2m and Des). CONCLUSIONS: PFOS exposure may alter placental development and function, causing intrauterine growth restriction via inhibiting placental 11beta-hydroxysteroid dehydrogenase 2.
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LA - eng

PT - Journal Article

DEP - 20160122

PL - Netherlands

TA - Placenta

JT - Placenta

JID - 8006349

SB - IM

OTO - NOTNLM

OT - 11beta-hydroxysteroid dehydrogenase 2

OT - Gene expression
 OT - Glucocorticoid
 OT - PFOS
 OT - Perfluoroalkylated substances
 OT - Placenta
 EDAT- 2016/03/20 06:00
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 PHST- 2016/01/22 [aheadofprint]
 AID - S0143-4004(16)30010-8 [pii]
 AID - 10.1016/j.placenta.2016.01.010 [doi]
 PST - ppublish
 SO - Placenta. 2016 Mar;39:125-33. doi: 10.1016/j.placenta.2016.01.010. Epub 2016 Jan 22.

 PMID- 26800430
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160405
 IS - 1615-9861 (Electronic)
 IS - 1615-9853 (Linking)
 VI - 16
 IP - 7
 DP - 2016 Apr
 TI - Designed synthesis of fluorous-functionalized magnetic mesoporous microspheres for specific enrichment of phosphopeptides with fluorous derivatization.
 PG - 1051-8
 LID - 10.1002/pmic.201500323 [doi]
 AB - In this work, for the first time, perfluorinated magnetic mesoporous microspheres were designed and synthesized for the highly specific enrichment of fluorous-derivatized phosphopeptides through the unique fluorine-fluorine interactions. The perfluorinated magnetic mesoporous microspheres were prepared through a surfactant-mediated one-pot approach and successfully applied to the selective extraction of fluorous-derivatized phosphopeptides from beta-casein tryptic digest, protein mixtures, and human serum. Thanks to the hydrophilic silanol groups exposed on the surface, perfluorinated groups modified in the pore channels and the magnetic cores, the fluorous-functionalized magnetic microspheres exhibited excellent dispersibility, specificity toward fluorous-derivatized phosphopeptides while facilitated separation procedures. The novel composites achieved a high selectivity of 1:1000 toward nonphosphorylated peptides and proved to be practicable in the enrichment of endogenous phosphopeptides in the human serum sample.
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 LA - eng
 PT - Journal Article
 DEP - 20160316
 PL - Germany
 TA - Proteomics
 JT - Proteomics
 JID - 101092707
 SB - IM
 OTO - NOTNLM
 OT - Enrichment
 OT - Fluorous proteomics
 OT - Fluorous solid-phase extraction
 OT - Functionalized magnetic mesoporous microspheres
 OT - Mass spectrometry
 OT - Technology
 EDAT- 2016/01/23 06:00
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 CRDT- 2016/01/23 06:00
 PHST- 2015/08/12 [received]
 PHST- 2015/12/24 [revised]
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 PHST- 2016/03/16 [aheadofprint]
 AID - 10.1002/pmic.201500323 [doi]
 PST - ppublish
 SO - Proteomics. 2016 Apr;16(7):1051-8. doi: 10.1002/pmic.201500323. Epub 2016 Mar 16.

 PMID- 26993749
 OWN - NLM
 STAT- Publisher
 DA - 20160412
 LR - 20160412
 IS - 1096-0295 (Electronic)
 IS - 0273-2300 (Linking)
 VI - 77
 DP - 2016 Mar 15
 TI - Influence of the uncertainty in the validation of PBPK models: A case-study for PFOS and PFOA.
 PG - 230-239
 LID - S0273-2300(16)30054-X [pii]
 LID - 10.1016/j.yrtph.2016.03.009 [doi]
 AB - Physiologically-based pharmacokinetic (PBPK) models are mathematical representations of the human body aimed at describing the time course distribution of chemicals in human tissues. Since parameterization of PBPK models is based on empirical estimation and experimental data, simulation results may

have high degree of uncertainty. As a consequence, the reliability of model validation is highly affected. In this study, the parametric uncertainty associated with PBPK models developed for perfluorooctane sulfonic acid (PFOS) and perfluorooctanoic acid (PFOA) were analyzed and the different validation approaches were discussed for a case-study in Tarragona County (NE of Spain). Physicochemical parameters and dietary intake of PFOS and PFOA were estimated from previous investigations performed in Tarragona County. A sensitivity analysis (SA) was performed to understand the degree of influence of input parameters on the final outcomes. The uncertainty of the PBPK models' outcome was assessed by propagating the parametric uncertainty using the Latin Hypercube Sampling (LHS) technique. The elimination constants (T_m and K_t) as well as the Free fraction and the Intake, were the most influential parameters according to the SA results, being up to 83% for PFOS and 99.9% for PFOA. The validation of the PBPK model, which was performed using different approaches, showed clear discrepancies in the visual validation when compared with the statistical analysis.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20160315

TA - Regul Toxicol Pharmacol

JT - Regulatory toxicology and pharmacology : RTP

JID - 8214983
 OTO - NOTNLM
 OT - Model validation
 OT - Perfluorooctane sulfonic acid (PFOS)
 OT - Perfluorooctanoic acid (PFOA)
 OT - Physiologically based pharmacokinetic (PBPK) model
 OT - Uncertainty analysis
 EDAT- 2016/03/20 06:00
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 PHST- 2016/03/08 [revised]
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 AID - S0273-2300(16)30054-X [pii]
 AID - 10.1016/j.yrtph.2016.03.009 [doi]
 PST - aheadofprint
 SO - Regul Toxicol Pharmacol. 2016 Mar 15;77:230-239. doi:
 10.1016/j.yrtph.2016.03.009.

PMID- 26943602
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160317
 IS - 2191-0308 (Electronic)
 IS - 0048-7554 (Linking)
 VI - 31
 IP - 1
 DP - 2016 Mar 1
 TI - Pilot-scale UV/H2O2 study for emerging organic contaminants decomposition.
 PG - 71-4
 LID - 10.1515/reveh-2016-0008 [doi]
 LID - /j/reveh.2016.31.issue-1/reveh-2016-0008/reveh-2016-0008.xml [pii]
 AB - Human behaviors including consumption of drugs and use of personal care products, climate change, increased international travel, and the advent of water reclamation for direct potable use have led to the introduction of significant amounts of emerging organic contaminants into the aqueous environment. In addition, the lower detection limits associated with improved scientific methods of chemical analysis have resulted in a recent increase in documented incidences of these contaminants which previously were not routinely monitored in water. Such contaminants may cause known or suspected adverse ecological and/or human health effects at very low concentrations. Conventional drinking water treatment processes may not effectively remove these organic contaminants. Advanced oxidation process (AOP) is a promising treatment process for the removal of most of these emerging organic contaminants, and has been accepted worldwide as a suitable treatment process. In this study, different groups of emerging contaminants were studied for decomposition efficiency using pilot-scale UV/H2O2 oxidation setup, including EDCs, PPCPs, taste and odor (T&O), and perfluorinated compounds. Results found that MP UV/H2O2 AOP was efficient in removing all the

selected contaminants except perfluorinated compounds. Study of the kinetics of the process showed that both light absorption and quantum yield of each compound affected the decomposition performance. Analysis of water quality parameters of the treated water indicated that the outcome of both UV photolysis and UV/H₂O₂ processes can be affected by changes in the feed water quality.

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FAU - Xing, Yongjie

AU - Xing Y

LA - eng

PT - Journal Article

PL - Germany

TA - Rev Environ Health

JT - Reviews on environmental health

JID - 0425754

SB - IM

EDAT- 2016/03/05 06:00

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AID - 10.1515/reveh-2016-0008 [doi]

AID - /j/reveh.ahead-of-print/reveh-2016-0008/reveh-2016-0008.xml [pii]

PST - ppublish

SO - Rev Environ Health. 2016 Mar 1;31(1):71-4. doi: 10.1515/reveh-2016-0008.

PMID- 26947748

OWN - NLM

STAT- In-Data-Review

DA - 20160307

LR - 20160310

IS - 2045-2322 (Electronic)

IS - 2045-2322 (Linking)

VI - 6

DP - 2016

TI - Spatial distribution and source apportionment of PFASs in surface sediments from five lake regions, China.

PG - 22674

LID - 10.1038/srep22674 [doi]

AB - Perfluoroalkyl substances (PFASs) have been found in environment globally. However, studies on PFAS occurrence in sediments of lakes or reservoirs remain relatively scarce. In this study, two hundred and sixty-two surface sediment samples were collected from forty-eight lakes and two reservoirs all over China. Average PFAS concentrations in surface sediments from each lake or reservoir varied from 0.086 ng/g dw to 5.79 ng/g dw with an average of 1.15 ng/g dw. Among five lake regions, average PFAS concentrations for the lakes from Eastern Plain Region were the highest. Perfluorooctanoic acid, perfluoroundecanoic acid and perfluorooctane sulfonic acid (PFOS) were the predominant PFASs in surface sediments. The significant positive correlations between PFAS concentrations and total organic carbon, total nitrogen and total phosphorus contents in sediments revealed the influences of sedimentary characteristics on PFAS occurrence. A two-dimensional hierarchical cluster analysis heat map was depicted to analyze the possible origins of sediments and individual PFAS. The food-packaging, textile, electroplating, firefighting and semiconductor industry emission sources and the precious metals and coating industry emission sources were identified as the main sources by two receptor models, with contributions of 77.7 and 22.3% to the total concentrations of C4-C14- perfluoroalkyl carboxylic acids and PFOS, respectively.

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LA - eng

PT - Journal Article

DEP - 20160307
PL - England
TA - Sci Rep
JT - Scientific reports
JID - 101563288
SB - IM
PMC - PMC4780192
OID - NLM: PMC4780192
EDAT- 2016/03/08 06:00
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AID - srep22674 [pii]
AID - 10.1038/srep22674 [doi]
PST - epublish
SO - Sci Rep. 2016 Mar 7;6:22674. doi: 10.1038/srep22674.

PMID- 27037875
OWN - NLM

STAT- Publisher

DA - 20160402

LR - 20160403

IS - 1879-1026 (Electronic)

IS - 0048-9697 (Linking)

VI - 557-558

DP - 2016 Mar 30

TI - Electrocoagulation mechanism of perfluorooctanoate (PFOA) on a zinc anode:
Influence of cathodes and anions.

PG - 542-550

LID - S0048-9697(16)30538-1 [pii]

LID - 10.1016/j.scitotenv.2016.03.114 [doi]

AB - Batch experiments were conducted to investigate the effects of cathode materials and anions (Cl⁻, SO₄²⁻, NO₃⁻, and CO₃²⁻/HCO₃⁻) on perfluorooctanoate (PFOA) removal in electrocoagulation process using zinc anode. The results indicated that the hydroxide flocs generated in-situ in the electrocoagulation process using the stainless steel rod as cathode were more effective than those using aluminum rod as cathode for the removal of PFOA after 20min of electrocoagulation at a current density of 0.5mA/cm². Hydroxide flocs generated in-situ in the electrocoagulation in the presence of Cl⁻/NO₃⁻ could effectively remove PFOA from aqueous solution with the removal ratios of 99.7%/98.1% and 98.9%/97.3% using stainless steel rod and aluminum rod as cathode, respectively. However, the PFOA removal ratios were 96.2%/4.1% and 7.4%/4.6% using stainless steel rod and aluminum rod as cathode, respectively, in the presence of SO₄²⁻ and CO₃²⁻/HCO₃⁻. The different removal ratios of PFOA during the electrocoagulation process were primarily due to the fact that the hydroxide flocs generated in-situ were different in the presence of diverse cathodes and anions. We firstly demonstrated that Zn_{0.70}Al_{0.30}(OH)₂(CO₃)_{0.15}·xH₂O and ZnO generated in-situ in the

electrocoagulation process (except for $\text{CO}_3^{2-}/\text{HCO}_3^-$) using zinc anode and aluminum/stainless steel rod cathode governed the sorption of PFOA. The adsorbent hydroxide flocs in-situ generated in the presence of Cl^- could effectively remove PFOA from aqueous solution containing $\text{CO}_3^{2-}/\text{HCO}_3^-$ anion at the initial hydroxide flocs concentration of 2000mgL^{-1} . These results provided an effective and alternative method to remove PFOA from aqueous solution containing $\text{CO}_3^{2-}/\text{HCO}_3^-$ anion.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20160330

TA - Sci Total Environ

JT - The Science of the total environment

JID - 0330500

OTO - NOTNLM

OT - Anions

OT - Cathode materials

OT - Electrocoagulation

OT - Hydroxide flocs

OT - Mechanisms
 OT - PFOA
 EDAT- 2016/04/03 06:00
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 AID - S0048-9697(16)30538-1 [pii]
 AID - 10.1016/j.scitotenv.2016.03.114 [doi]
 PST - aheadofprint
 SO - Sci Total Environ. 2016 Mar 30;557-558:542-550. doi:
 10.1016/j.scitotenv.2016.03.114.

 PMID- 26950632
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160402
 IS - 1879-1026 (Electronic)
 IS - 0048-9697 (Linking)
 VI - 554-555
 DP - 2016 Jun 1
 TI - Behaviors of N-ethyl perfluorooctane sulfonamide ethanol (N-EtFOSE) in a
 soil-earthworm system: Transformation and bioaccumulation.
 PG - 186-91
 LID - 10.1016/j.scitotenv.2016.02.180 [doi]
 LID - S0048-9697(16)30391-6 [pii]
 AB - N-ethyl perfluorooctane sulfonamido ethanol (N-EtFOSE) is a typical precursor of
 perfluorooctane sulfonate (PFOS). In this study, the behaviors of N-EtFOSE in a
 soil-earthworm system, including biodegradation in soil and bioaccumulation and
 biotransformation in earthworms (*Eisenia fetida*) were investigated. N-EtFOSE
 could be biodegraded in soil and biotransformed in earthworms to several
 metabolites, including n-ethylperfluorooctane sulfonamide acetate (N-EtFOSAA),
 perfluorooctane sulfonamide acetate (FOSAA), perfluorooctane sulfonamide (FOSA)
 and PFOS, with N-EtFOSAA as the predominant intermediate and PFOS as the terminal
 product in both soil and earthworm. The uptake rate coefficients (k_u , 0.746 goc
 gdw⁻¹d⁻¹), degradation rate constant in soil (k_0 , 0.138d⁻¹) and the
 biota-to-soil accumulation factor (BSAF, 0.523 goc gdw⁻¹) of N-EtFOSE were
 estimated. For N-EtFOSE, N-EtFOSAA, FOSAA, FOSA and PFOS, their loss rate
 constants in earthworms were in the range of 0.467-30.2 (alpha) and 0.006-0.415
 (beta) d⁻¹, respectively. The results provided important information about the
 behaviors of N-EtFOSE in the soil-earthworm system.
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LA - eng

PT - Journal Article

DEP - 20160305

PL - Netherlands

TA - Sci Total Environ

JT - The Science of the total environment

JID - 0330500

SB - IM

OTO - NOTNLM

OT - Bioaccumulation

OT - Biotransformation

OT - Earthworm

OT - N-EtFOSE

OT - Soil

EDAT- 2016/03/08 06:00

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AID - S0048-9697(16)30391-6 [pii]

AID - 10.1016/j.scitotenv.2016.02.180 [doi]

PST - ppublish

SO - Sci Total Environ. 2016 Jun 1;554-555:186-91. doi: 10.1016/j.scitotenv.2016.02.180. Epub 2016 Mar 5.

PMID- 26844784

OWN - NLM

STAT- In-Data-Review

DA - 20160305

IS - 1096-0333 (Electronic)

IS - 0041-008X (Linking)

VI - 295

DP - 2016 Mar 15

TI - Role of miR-155 in fluorooctane sulfonate-induced oxidative hepatic damage via the Nrf2-dependent pathway.

PG - 85-93

LID - 10.1016/j.taap.2016.01.023 [doi]

LID - S0041-008X(16)30023-0 [pii]

AB - Studies demonstrated that perfluorooctane sulfonate (PFOS) tends to accumulate in the liver and is capable to cause hepatomegaly. In the present study, we investigated the roles of miR-155 in PFOS-induced hepatotoxicity in SD rats and HepG2 cells. Male SD rats were orally administrated with PFOS at 1 or 10mg/kg/day for 28days while HepG2 cells were treated with 0-50μM of PFOS for 24h or 50μM of PFOS for 1, 3, 6, 12 or 24h, respectively. We found that PFOS significantly increased the liver weight and serum alanine transaminase (ALT) and aspartate amino transferase (AST) levels in rats. Morphologically, PFOS caused actin filament remodeling and endothelial permeability changes in the liver. Moreover, PFOS triggered reactive oxygen species (ROS) generation and induced apoptosis in both in vivo and in vitro assays. Immunoblotting data showed that NF-E2-related factor-2 (Nrf2) expression and activation and its target genes were all suppressed by PFOS in the liver and HepG2 cells. However, PFOS significantly increased miR-155 expression. Further studies showed that pretreatment of HepG2 cells with catalase significantly decreased miR-155 expression and substantially increased Nrf2 expression and activation, resulting in reduction of PFOS-induced cytotoxicity and oxidative stress. Taken together, these results indicated that miR-155 plays an important role in the PFOS-induced hepatotoxicity by disrupting Nrf2/ARE signaling pathway.

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LA - eng

PT - Journal Article

DEP - 20160201

PL - United States

TA - Toxicol Appl Pharmacol

JT - Toxicology and applied pharmacology

JID - 0416575

SB - IM

OTO - NOTNLM

OT - Hepatotoxicity

OT - Nrf2

OT - Oxidative stress

OT - PFOS

OT - miR155

EDAT- 2016/02/05 06:00

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PHST- 2016/02/01 [aheadofprint]

AID - S0041-008X(16)30023-0 [pii]

AID - 10.1016/j.taap.2016.01.023 [doi]

PST - ppublish

SO - Toxicol Appl Pharmacol. 2016 Mar 15;295:85-93. doi: 10.1016/j.taap.2016.01.023.
Epub 2016 Feb 1.

PMID- 26772051

OWN - NLM

STAT- In-Data-Review

DA - 20160217

IS - 1096-0333 (Electronic)

IS - 0041-008X (Linking)

VI - 294

DP - 2016 Mar 1

TI - Effects of defined mixtures of persistent organic pollutants (POPs) on multiple cellular responses in the human hepatocarcinoma cell line, HepG2, using high

content analysis screening.

PG - 21-31

LID - 10.1016/j.taap.2016.01.001 [doi]

LID - S0041-008X(16)30001-1 [pii]

AB - Persistent organic pollutants (POPs) are toxic substances, highly resistant to environmental degradation, which can bio-accumulate and have long-range atmospheric transport potential. Most studies focus on single compound effects, however as humans are exposed to several POPs simultaneously, investigating exposure effects of real life POP mixtures on human health is necessary. A defined mixture of POPs was used, where the compound concentration reflected its contribution to the levels seen in Scandinavian human serum (total mix). Several sub mixtures representing different classes of POPs were also constructed. The perfluorinated (PFC) mixture contained six perfluorinated compounds, brominated (Br) mixture contained seven brominated compounds, chlorinated (Cl) mixture contained polychlorinated biphenyls and also p,p'-dichlorodiphenyldichloroethylene, hexachlorobenzene, three chlordanes, three hexachlorocyclohexanes and dieldrin. Human hepatocarcinoma (HepG2) cells were used for 2h and 48h exposures to the seven mixtures and analysis on a CellInsight NXT High Content Screening platform. Multiple cytotoxic endpoints were investigated: cell number, nuclear intensity and area, mitochondrial mass and membrane potential (MMP) and reactive oxygen species (ROS). Both the Br and Cl mixtures induced ROS production but did not lead to apoptosis. The PFC mixture induced ROS production and likely induced cell apoptosis accompanied by the dissipation of MMP. Synergistic effects were evident for ROS induction when cells were exposed to the PFC+Br mixture in comparison to the effects of the individual mixtures. No significant effects were detected in the Br+Cl, PFC+Cl or total mixtures, which contain the same concentrations of chlorinated compounds as the Cl mixture plus additional compounds; highlighting the need for further exploration of POP mixtures in risk assessment.

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 LA - eng
 PT - Journal Article
 DEP - 20160107
 PL - United States
 TA - Toxicol Appl Pharmacol
 JT - Toxicology and applied pharmacology
 JID - 0416575
 SB - IM
 OTO - NOTNLM
 OT - Cytotoxicity
 OT - High content analysis
 OT - Mixtures
 OT - Persistent organic pollutants
 EDAT- 2016/01/17 06:00
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 PHST- 2016/01/07 [aheadofprint]
 AID - S0041-008X(16)30001-1 [pii]
 AID - 10.1016/j.taap.2016.01.001 [doi]
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 SO - Toxicol Appl Pharmacol. 2016 Mar 1;294:21-31. doi: 10.1016/j.taap.2016.01.001. Epub 2016 Jan 7.

 PMID- 27018931
 OWN - NLM
 STAT- In-Data-Review
 DA - 20160408
 IS - 1879-3185 (Electronic)
 IS - 0300-483X (Linking)
 VI - 347-349
 DP - 2016 Mar 10
 TI - Developmental perfluorooctane sulfonate exposure results in tau hyperphosphorylation and beta-amyloid aggregation in adults rats: Incidence for link to Alzheimer's disease.
 PG - 40-6
 LID - 10.1016/j.tox.2016.03.003 [doi]
 LID - S0300-483X(16)30021-X [pii]
 AB - With regard to the defects of the cognitive function observed after developmental

exposure to perfluorooctane sulfonate (PFOS), and earlier studies on the developmental neurotoxicology, the aim of this study was to investigate the role of developmental PFOS exposure in neurodegenerative disorders in later life. Two pathological hallmarks of Alzheimer's disease (AD), Tau hyperphosphorylation and beta-amyloid (A β) aggregation, were examined. SD rats were exposed to PFOS during only prenatal and/or postnatal period. Tau mRNA and protein levels were elevated by PFOS exposure. The phosphorylation of Tau at S199, T231 and S396 sites were also increased. Besides, PFOS exposure increased the A β 1-42 levels, as well as the amyloid precursor protein (APP) regulation. The prenatal PFOS exposure caused alterations in the involved proteins at comparable levels with the postnatal and both prenatal and postnatal exposure. Thus, it has raised some evidence that early PFOS exposure can affect processes linked to neurodegeneration, enhancing the AD pathological risk. And PFOS exposures in early life may be of particular etiologic importance of neurodegenerative diseases.

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LA - eng

PT - Journal Article

DEP - 20160324

PL - Ireland

TA - Toxicology

JT - Toxicology

JID - 0361055

SB - IM

OTO - NOTNLM

OT - Alzheimer's disease

OT - Amyloid protein

OT - Learning and memory

OT - PFOS

OT - Tau phosphorylation

EDAT- 2016/03/29 06:00

MHDA- 2016/03/29 06:00

CRDT- 2016/03/29 06:00

PHST- 2016/01/02 [received]

PHST- 2016/03/21 [revised]

PHST- 2016/03/23 [accepted]

PHST- 2016/03/24 [aheadofprint]

AID - S0300-483X(16)30021-X [pii]

AID - 10.1016/j.tox.2016.03.003 [doi]

PST - ppublish

SO - Toxicology. 2016 Mar 10;347-349:40-6. doi: 10.1016/j.tox.2016.03.003. Epub 2016
Mar 24.

PMID- 26774262

OWN - NLM

STAT- In-Data-Review

DA - 20160216

IS - 1879-2448 (Electronic)

IS - 0043-1354 (Linking)

VI - 91

DP - 2016 Mar 15

TI - Use of strong anion exchange resins for the removal of perfluoroalkylated
substances from contaminated drinking water in batch and continuous pilot plants.

PG - 137-46

LID - 10.1016/j.watres.2015.12.039 [doi]

LID - S0043-1354(15)30437-1 [pii]

AB - In recent years abnormally high levels of perfluoroalkylated substances (PFAS)
have been detected both in surface and underground water sampled in an area
covering approximately 150 square kilometers in the Veneto region (Italy)
indicating the presence of a pollution point source (fluorochemicals production
plant). Adsorption on granular activated carbon is an emergency measure which is
poorly effective requiring frequent replacement. This work focuses on the

application of three strong anion exchange resins (Purolite(R) A520E, A600E and A532E) for the removal of traces of PFOA, PFOS, PFBA and PFBS (concentration of hundreds of ng L⁻¹) from drinking water. This technology is attractive for the possibility of reusing resins after an in-situ regeneration step. A strong relationship between the hydrophobicity of the exchange functional group of the resin and its capacity in removing PFAS exists. A600E (non hydrophobic) and A520E (fairly hydrophobic) show a reduced sorption capacity compared to A532E (highly hydrophobic). While A600E and A520E can be regenerated with solvent-less dilute solutions of non-toxic NH₄Cl and NH₄OH, A532E requires concentrated solutions of methanol or ethanol and 1% NH₄Cl and for the sake of this work it was regarded as non-regenerable. The volume of regeneration effluents requiring incineration can be efficiently reduced by more than 96.5% by using reverse osmosis coupled with under-vacuum evaporation. Transmission electron analysis on saturated resins showed that large molecular macro-aggregates of PFAS can form in the intraparticle pores of resin indicating that ion exchange is not the only mechanism involved in PFAS removal.

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LA - eng

PT - Journal Article

DEP - 20151230

PL - England

TA - Water Res

JT - Water research

JID - 0105072

SB - IM

OTO - NOTNLM

OT - Anion exchange resin

OT - Granular activated carbon

OT - Ion exchange
 OT - PFAS
 OT - Removal
 EDAT- 2016/01/18 06:00
 MHDA- 2016/01/18 06:00
 CRDT- 2016/01/18 06:00
 PHST- 2015/09/21 [received]
 PHST- 2015/11/27 [revised]
 PHST- 2015/12/23 [accepted]
 PHST- 2015/12/30 [aheadofprint]
 AID - S0043-1354(15)30437-1 [pii]
 AID - 10.1016/j.watres.2015.12.039 [doi]
 PST - ppublish
 SO - Water Res. 2016 Mar 15;91:137-46. doi: 10.1016/j.watres.2015.12.039. Epub 2015 Dec 30.

 PMID- 26990839
 OWN - NLM
 STAT- Publisher
 DA - 20160318
 LR - 20160319
 IS - 1879-2448 (Electronic)
 IS - 0043-1354 (Linking)
 VI - 95
 DP - 2016 Mar 10
 TI - Poly- and perfluoroalkyl substances in wastewater: Significance of unknown precursors, manufacturing shifts, and likely AFFF impacts.
 PG - 142-149
 LID - S0043-1354(16)30114-2 [pii]
 LID - 10.1016/j.watres.2016.02.055 [doi]
 AB - In late 2014, wastewater effluent samples were collected from eight treatment plants that discharge to San Francisco (SF) Bay in order to assess poly- and perfluoroalkyl substances (PFASs) currently released from municipal and industrial sources. In addition to direct measurement of twenty specific PFAS analytes, the total concentration of perfluoroalkyl acid (PFAA) precursors was also indirectly measured by adapting a previously developed oxidation assay. Effluent from six municipal treatment plants contained similar amounts of total PFASs, with highest median concentrations of PFHxA (24 ng/L), followed by PFOA (23 ng/L), PFBA (19 ng/L), and PFOS (15 ng/L). Compared to SF Bay municipal wastewater samples collected in 2009, the short chain perfluorinated carboxylates PFBA and PFHxA rose significantly in concentration. Effluent samples from two treatment plants contained much higher levels of PFASs: over two samplings, wastewater from one municipal plant contained an average of 420 ng/L PFOS and wastewater from an airport industrial treatment plant contained 560 ng/L PFOS, 390 ng/L 6:2 FtS, 570 ng/L PFPeA, and 500 ng/L PFHxA. The elevated levels observed in effluent samples from these two plants are likely related to aqueous film forming foam (AFFF) sources impacting their influent; PFASs attributable to both current use and discontinued AFFF formulations were observed. Indirectly

measured PFAA precursor compounds accounted for 33%-63% of the total molar concentration of PFASs across all effluent samples and the PFAA precursors indicated by the oxidation assay were predominately short-chained. PFAS levels in SF Bay effluent samples reflect the manufacturing shifts towards shorter chained PFASs while also demonstrating significant impacts from localized usage of AFFF.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20160310

TA - Water Res

JT - Water research

JID - 0105072

OTO - NOTNLM

OT - Aqueous film forming foam (AFFF)

OT - Poly- and perfluoroalkyl substances (PFASs)

OT - San Francisco Bay

OT - Total oxidizable precursor method

OT - Wastewater effluent

EDAT- 2016/03/19 06:00

MHDA- 2016/03/19 06:00

CRDT- 2016/03/19 06:00

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PHST- 2016/02/05 [revised]

PHST- 2016/02/27 [accepted]

AID - S0043-1354(16)30114-2 [pii]

AID - 10.1016/j.watres.2016.02.055 [doi]

PST - aheadofprint

SO - Water Res. 2016 Mar 10;95:142-149. doi: 10.1016/j.watres.2016.02.055.

PMID- 26648086

OWN - NLM

STAT- In-Data-Review

DA - 20160303

IS - 1097-0061 (Electronic)

IS - 0749-503X (Linking)

VI - 33

IP - 3

DP - 2016 Mar

TI - Cloning and evaluation of different constitutive promoters in the oleaginous yeast *Rhodospiridium toruloides*.

PG - 99-106

LID - 10.1002/yea.3145 [doi]

AB - The oleaginous yeast *Rhodospiridium toruloides* is an unconventional yeast species that can accumulate a high content of lipids. Because it belongs to the basidiomycetous group of fungus, limited tools and functional elements are available for genetic engineering of *R. toruloides* and related red yeasts. Here we report the functional evaluation of five constitutive promoters from this yeast. We assembled a reporter gene expression cassette, consisting of a promoter, the hygromycin gene (HYG) and the nos terminator, and inserted it into the binary vector pZPK. Hygromycin-resistant transformants were obtained when *R. toruloides* cells were co-cultured with *Agrobacterium tumefaciens* AGL1 cells harbouring the engineered vector. Genomic integration of the reporter cassette was verified by successful amplification of target DNA fragments. Quantitative PCR analysis suggested that the transformant had only one copy of the reporter cassette. The strength of these promoters was demonstrated at the phenotypic level on the hygromycin-gradient plate and at the transcriptional level by real-time quantitative PCR. It was found that the strengths of these promoters varied no more than five-fold and followed a decreasing sequence of PPGI, PPGK, PFBA, PTPI, and PGPD. This study established new genetic elements for the construction of superior *R. toruloides* strains to produce advanced biofuels and related chemicals. Copyright (c) 2015 John Wiley & Sons, Ltd.

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LA - eng
PT - Journal Article
DEP - 20160114
PL - England
TA - Yeast
JT - Yeast (Chichester, England)
JID - 8607637
SB - IM
OTO - NOTNLM
OT - Rhodosporidium toruloides
OT - genetic engineering
OT - promoter
OT - transformation
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PHST- 2015/11/27 [accepted]
PHST- 2016/01/14 [aheadofprint]
AID - 10.1002/yea.3145 [doi]
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SO - Yeast. 2016 Mar;33(3):99-106. doi: 10.1002/yea.3145. Epub 2016 Jan 14.